Jan Delaval please

Access DB# 67522

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabiha Qazi Examiner #: 74141 Date: 5/25/02
Art Unit: 1616 Phone Number 30.5-3910 Serial Number: 09/893,324
Mail Box and Bldg/Room Location: 2019 CM1 3B07. Results Format Preferred (circle): (PAPER) DISK E-MAIL

If mor than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Alkyl ether modified polycyclic compds having a terminal phenol + uses

Inventors (please provide full names): Prokai et al.

Earliest Priority Filing Date: 6/27/01

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for a steroidal compd when ring A is unsaturated and containing an alkyl ether at 17-position of D ring.
e.g. 1,3,5(10) triene-3-ol-17-alkyl ether estradiol.

Please see attached Root

Thank you

Jan Delaval
Reference Librarian
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

****

STAFF USE ONLY

Searcher: Jan
Searcher Phone #: 4498
Searcher Location:
Date Searcher Picked Up: 5/29/02
Date Completed: 5/29/02
Searcher Prep & Review Time:
Clerical Prep Time: 15
Online Time: 140

Type of Search

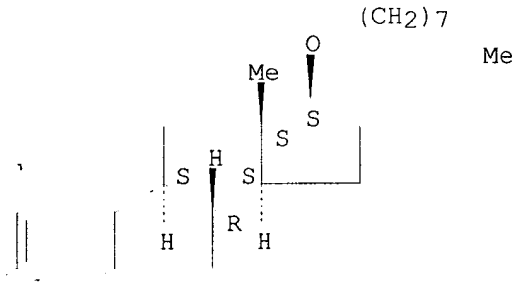
NA Sequence (#)
AA Sequence (#) 0
Structure (#)
Bibliographic
Litigation
Fulltext
Patent Family
Other

Vendors and cost where applicable

STN
Dialog
Questel/Orbit
Dr.Link
Lexis/Nexis
Sequence Systems ✓
WWW/Internet
Other (specify)

PTO-1590 (8-01)

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 11:20:53 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:   27 MAY 2002  HIGHEST RN 422267-53-6
DICTIONARY FILE UPDATES:  27 MAY 2002  HIGHEST RN 422267-53-6

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Calculated physical property data is now available.  See HELP PROPERTIES
for more information.  See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d ide can tot l21

L21  ANSWER 1 OF 5  REGISTRY  COPYRIGHT 2002 ACS
RN   319427-07-1  REGISTRY
CN   Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17.beta.)- (9CI)  (CA INDEX
     NAME)
FS   STEREOSEARCH
MF   C26 H40 O2
SR   CA
LC   STN Files:   CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
```

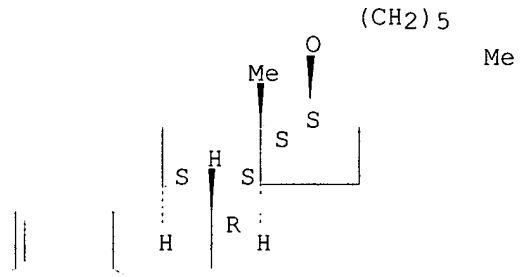



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               3 REFERENCES IN FILE CA (1967 TO DATE)
               3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE   1:  136:85991

REFERENCE   2:  135:221441

REFERENCE   3:  134:101056

L21  ANSWER 2 OF 5  REGISTRY  COPYRIGHT 2002 ACS
RN   319427-06-0  REGISTRY
CN   Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17.beta.)- (9CI)  (CA INDEX
     NAME)
```

Jan Delaval
Reference Librarian
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

FS STEREOSEARCH
MF **C24 H36 O2**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

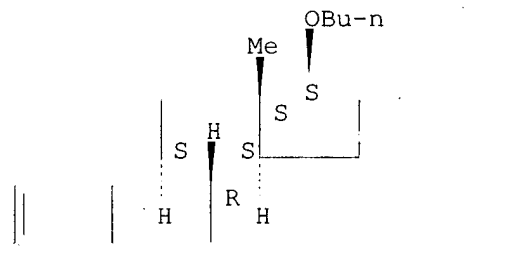
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2002 ACS
RN **319427-05-9** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C22 H32 O2**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

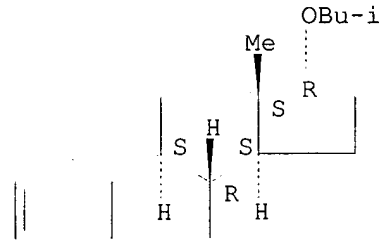
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2002 ACS

RN 119309-39-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17.alpha.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17.alpha.-Isobutylestradiol
FS STEREOSEARCH
MF **C22 H32 O2**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

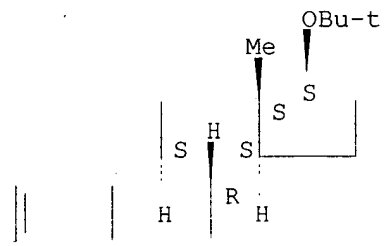
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:29367

REFERENCE 2: 110:121535

L21 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2002 ACS
RN 38781-59-8 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C22 H32 O2**
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 85:154233

REFERENCE 2: 80:121187

REFERENCE 3: 77:101990

=> d his l21-

```
     (FILE 'REGISTRY' ENTERED AT 11:12:06 ON 29 MAY 2002)
L21           5 S L15,L20
                SEL RN
L22           0 S E19-E23/CRN

     FILE 'HCAOLD' ENTERED AT 11:20:06 ON 29 MAY 2002
L23           0 S L21

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:20:07 ON 29 MAY 2002
L24           1 S L21

     FILE 'HCAPLUS' ENTERED AT 11:20:18 ON 29 MAY 2002
L25           8 S L21
L26           3 S L1-L3 AND L25
L27           8 S L25,L26

     FILE 'REGISTRY' ENTERED AT 11:20:53 ON 29 MAY 2002
```

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 11:21:06 ON 29 MAY 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 11:21:06 ON 29 MAY 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

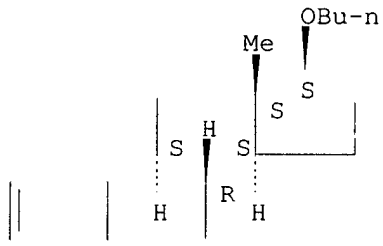
=> d l24 bib abs hitstr

L24 ANSWER 1 OF 1 USPATFULL
AN 2002:61264 USPATFULL
TI Alkyl ether modified polycyclic compounds having a terminal phenol and uses for protection of cells
IN Prokai, Laszlo, Gainesville, FL, UNITED STATES
Simpkins, James W., Fort Worth, TX, UNITED STATES
PI US 2002035100 A1 20020321
AI US 2001-893324 A1 20010627 (9)
PRAI US 2000-214077P 20000627 (60)
DT Utility
FS APPLICATION
LREP BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618
CLMN Number of Claims: 46
ECL Exemplary Claim: 1
DRWN 5 Drawing Page(s)
LN.CNT 951
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Methods and compositions are provided for achieving a cytoprotective effect by selecting a polycyclic compound with a phenol group at one end of the molecule and a carbon ring at the other such that an alkyl ether functional group in which the alkyl group has a formula C.sub.nH.sub.2n+1 (where n is at least 3 and less than 20) is positioned on the carbon ring. The compound may be used to achieve a cytoprotective effect in cells and to retard the development of a degenerative condition in a subject suffering from a disease, trauma or aging.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **319427-05-9P**
(crystal structure)
RN 319427-05-9 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

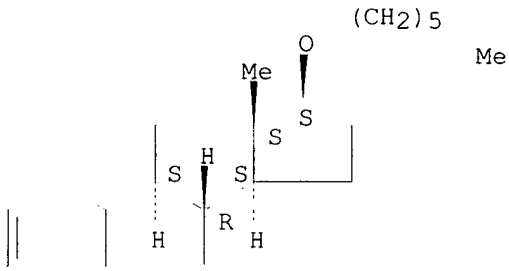
Absolute stereochemistry.



HO

IT **319427-06-0P 319427-07-1P**
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
RN 319427-06-0 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

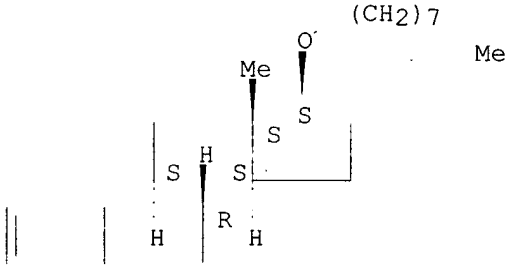
Absolute stereochemistry.



HO

RN 319427-07-1 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 11:21:16 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 29 May 2002 VOL 136 ISS 22
FILE LAST UPDATED: 27 May 2002 (20020527/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

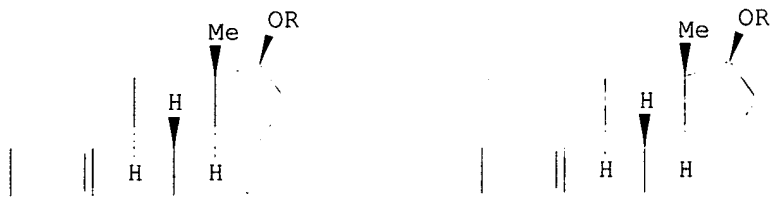
CAS roles have been modified effective December 16, 2001. Please
check your SDI profiles to see if they need to be revised. For
information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> d all hitstr tot l27

L27 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:10439 HCAPLUS
DN 136:85991
TI Preparation of 17.beta.-alkyl ether estradiol derivatives with cytoprotective activity of cells from degeneration through disease, trauma or aging
IN **Prokai, Laszlo; Simpkins, James W.**
PA University of Florida Research Foundation, Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000619	A2	20020103	WO 2001-US41170	20010627
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2002035100	A1	20020321	US 2001-893324	20010627
PRAI	US 2000-214077P	P	20000627		

GI



AB Cytoprotective compds. I (R = Me, Et, Pr, Bu, (CH2)5Me, or (CH2)7Me; R1 = OH) were prepd. in 50-75% yields from 17.beta.-estradiol. 17.beta.-Estradiol and benzyl halide in K2CO3 gave 93% yield of 3-benzyloxyestra-1,3,5(10)-trien-17.beta.-ol which was then alkylated with the appropriate alkyl halides in DMF and NaH yielding the 3-benzyloxy protected derivs. of I which were then deprotected via catalytic hydrogenation using ammonium formate in Pd/C. Thus compds. II (R = hexyl and octyl) were prepd. in 70 and 75% resp., and were neuroprotective to a similar extent at a concn. of 10 .mu.M and 1 .mu.M. Typical compns. contain approx. 0.01-95% by wt. of active ingredient and the percentage of active ingredient will depend upon the dosage form and mode of administration; an ED of the active agent as measured in the plasma of a subject may be in the range of 5pg/mL-5000pg/mL. Cytoprotective compds. I (R = OH; R1 = Bu, (CH2)7Me) were prepd. from 17.beta.-estradiol and Bu or octyl bromide in K2CO3 in 68 and 72% resp.

ST estradiol hydroxy alkylated deriv prepn cytoprotective compn; neuroprotective alkyl ether steroid prepn; crystal structure butoxyestratrienol

IT Steroids, preparation
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(alkylation of 17.beta.-OH or 3-OH; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Cytoprotective agents
(cardioprotective; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Nervous system
(degeneration; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Alkylation
(hydroxyalkylation; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Eye, disease
(macula, degeneration; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Crystal structure
(of 17.beta.-butoxyestra-1,3,5(10)-trien-3-ol)

IT Estrogen receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used as cytoprotective agents of cells from degeneration)

IT Anti-Alzheimer's agents
Anti-ischemic agents
Bone, disease
Drug delivery systems
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Osteoporosis
(therapeutic agents; prepn. of 17.beta.- or 3-alkyl ether derivs. of

estradiol used for cytoprotective activity of cells from degeneration)

IT **319427-05-9P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure)

IT 4954-12-5P 21830-24-0P 128805-68-5P 319427-03-7P 319427-04-8P
319427-06-0P 319427-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

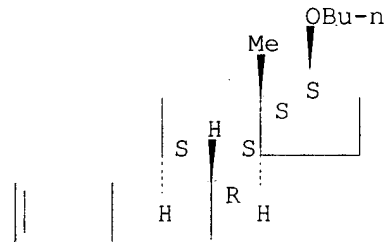
IT 50-28-2, 17.beta.-Estradiol, reactions 109-65-9, Butyl bromide 111-83-1, Octyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT 14982-15-1P 141318-37-8P 319426-98-7P 319426-99-8P 319427-00-4P 319427-01-5P 319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT **319427-05-9P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure)

RN 319427-05-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

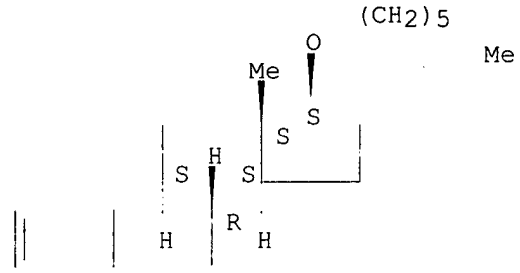
Absolute stereochemistry.



IT **319427-06-0P 319427-07-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

RN 319427-06-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

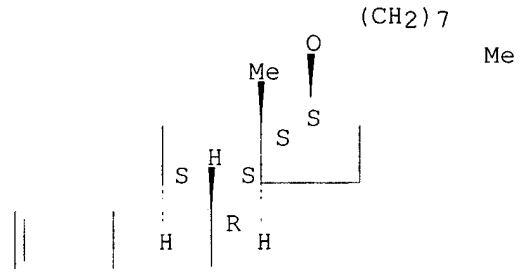
Absolute stereochemistry.



HO

RN 319427-07-1 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

L27 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:428147 HCAPLUS
DN 135:221441
TI Membrane fluidity effects of estratrienes
AU Liang, Y.; Belford, S.; Tang, F.; **Prokai, L.**; **Simpkins, J. W.**; Hughes, J. A.
CS Department of Pharmaceutics, University of Florida, Gainesville, FL, USA
SO Brain Research Bulletin (2001), 54(6), 661-668
CODEN: BRBUDU; ISSN: 0361-9230
PB Elsevier Science Inc.
DT Journal
LA English
CC 2-4 (Mammalian Hormones)
AB Estrogens have demonstrable neuroprotective effects. This fact has lead to the proposed use of estrogens for the prevention and/or treatment of Alzheimer's disease. The exact protective mechanism estrogens provide is not fully understood. In this report, a potential non-genomic mechanism for estratrienes involving alterations in membrane fluidity was studied. Steroids, such as estrogen, are known to be membrane-active and can alter the lipid packing. In this study the authors used fluorescent methodologies to address the effect of naturally occurring steroids (17.alpha.- and 17.beta.-estradiol, testosterone, and progesterone) and new estratriene analogs on membrane fluidity using liposomes and HT-22 hippocampal cells. The study's results indicate steroids, based on the estratriene nucleus, can modulate lipid packing as evidenced by (1) decreased membrane fusion events and (2) decreased membrane fluidity. The effects on the membrane were both time- and concn.-dependent. It was also demonstrated through rational design estratriene analogs can be synthesized with enhanced membrane effects. Finally, in a

glutamate-induced toxicity HT-22 model, the authors also demonstrated cellular protection with the estratriene-based mols. and analogs. The data suggest the plethora of cellular actions of estrogens may relate to or be influenced by membrane effects of the steroid.

ST cell membrane fluidity estratriene; estradiol membrane fluidity

IT Animal cell line
(HT-22; estratrienes effects on membrane fluidity)

IT Membrane, biological
(bilayer; estratrienes effects on membrane fluidity)

IT Liposomes
(estratrienes effects on membrane fluidity)

IT Phosphatidylethanolamines, biological studies
Phosphatidylserines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(estratrienes effects on membrane fluidity)

IT Brain
(hippocampus; estratrienes effects on membrane fluidity)

IT 57-88-5, Cholesterol, biological studies
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(estratrienes effects on membrane fluidity)

IT 50-28-2, 17.beta.-Estradiol, biological studies 53-63-4, Estra-1,3,5(10)-trien-3-ol 57-83-0, Progesterone, biological studies 57-91-0, 17.alpha.-Estradiol 58-22-0, Testosterone
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(estratrienes effects on membrane fluidity)

IT **319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(estratrienes effects on membrane fluidity)

IT 50-50-0, 17.beta.-Estradiol 3-benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(estratrienes effects on membrane fluidity)

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Abrami, L; J Cell Biol 1999, V147, P175 HCAPLUS
(2) Behl, C; Biochem Biophys Res Commun 1995, V216, P473 HCAPLUS
(3) Behl, C; Int J Vitam Nutr Res 1999, V69, P213 HCAPLUS
(4) Behl, C; Prog Neurobiol 1999, V57, P301 HCAPLUS
(5) Bodor, N; J Am Chem Soc 1989, V111, P3783 HCAPLUS
(6) Cowley, S; J Biol Chem 1997, V272(2), P19858
(7) Davy, A; J Neurochem 2000, V74, P676 HCAPLUS
(8) Dewar, M; J Am Chem Soc 1985, V107, P3902 HCAPLUS
(9) Dicko, A; Brain Res Bull 1999, V49, P401 HCAPLUS
(10) Golden, G; Life Sci 1999, V65, P1247 HCAPLUS
(11) Green, P; J Neurosci 1997, V17, P511 HCAPLUS
(12) Gridley, K; Mol Pharmacol 1998, V54, P874 HCAPLUS
(13) Gu, Q; J Physiol 1998, V506, P745 HCAPLUS
(14) Hayashi, H; Biochim Biophys Acta 2000, V1483, P81 HCAPLUS
(15) Henderson, V; Arch Neurol 1994, V51, P896 MEDLINE
(16) Holopainen, J; Chem Phys Lipids 1997, V88, P1 HCAPLUS
(17) Horvat, A; Experientia 1995, V51, P11 HCAPLUS
(18) Inestrosa, N; Mol Neurobiol 1998, V17, P73 HCAPLUS
(19) Kalman, J; Biol Psychiatry 1994, V35, P190 MEDLINE
(20) Kawas, C; Neurology 1997, V48, P1517 HCAPLUS
(21) Kawas, C; published erratum appears in Neurology 1998, V51(2), P654
(22) Keller, I; J Neurosci Res 1997, V50, P522
(23) Lakowicz, J; Principles of fluorescence spectroscopy 1986
(24) Lue, L; Am J Pathol 1999, V155, P853 MEDLINE

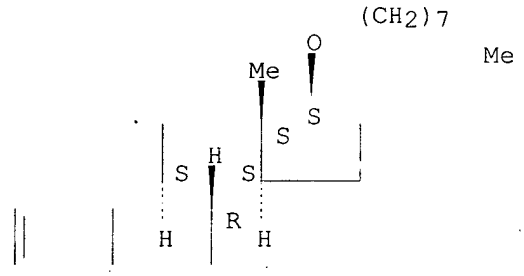
(25) Marra, C; Acta Physiol Pharmacol Ther, Latinoam 1998, V48, P8 MEDLINE
(26) Moosmann, B; Proc Natl Acad Sci 1999, V96, P8867 HCAPLUS
(27) Moss, R; Steroids 1999, V64, P14 HCAPLUS
(28) Muller, W; Amyloid 1998, V5, P10 HCAPLUS
(29) Pappas, T; FASEB J 1995, V9, P404 HCAPLUS
(30) Parikh, I; J Steroid Biochem 1987, V27, P185 HCAPLUS
(31) Pasenkiewicz-Gierula, M; Biochimie 1991, V73, P1311 HCAPLUS
(32) Pike, C; J Neurochem 1999, V72, P1552 HCAPLUS
(33) Raffy, S; Biophys J 1999, V76, P2072 HCAPLUS
(34) Saez, R; FEBS Lett 1995, V179, P311
(35) Schneider, L; Am J Med 1997, V103(3A), P46S MEDLINE
(36) Schneider, L; Ann NY Acad Sci 1997, V826, P317 HCAPLUS
(37) Sherwin, B; Neurology 1997, V48(suppl 7), PS21
(38) Simpkins, J; Am J Med 1997, V103(3A), P19S MEDLINE
(39) Simpkins, J; J Neurosurg 1997, V87, P724 HCAPLUS
(40) Smith, A; Hosp Pract P157
(41) Smith, A; Hosp Pract 1998, V33(3), P151 MEDLINE
(42) Verhagen, J; J Lipid Res 1996, V37, P1488 HCAPLUS
(43) Wong, M; J Neurosci 1992, V12, P3217 HCAPLUS
(44) Xiang, T; Biophys J 1998, V75, P2658 HCAPLUS
(45) Yang, J; Biophys J 1999, V76(1), P323 HCAPLUS

IT **319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(estratrienes effects on membrane fluidity)

RN 319427-07-1 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2002 ACS

AN 2000:820327 HCAPLUS

DN 134:101056

TI Synthesis and Biological Evaluation of 17.beta.-Alkoxyestra-1,3,5(10)-trienes as Potential Neuroprotectants Against Oxidative Stress

AU **Prokai, Laszlo**; Oon, Su-Min; Prokai-Tatrai, Katalin; Abboud, Khalil A.; **Simpkins, James W.**

CS Center for Drug Discovery College of Pharmacy Department of Anesthesiology College of Medicine and Center for Neurobiology of Aging College of Pharmacy, University of Florida, Gainesville, FL, 32610-0497, USA

SO Journal of Medicinal Chemistry (2001), 44(1), 110-114
CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

CC 32-3 (Steroids)
Section cross-reference(s): 1, 75

OS CASREACT 134:101056

AB 17.beta.-O-Alkyl ethers (Me, Et, Pr, Bu, hexyl, and octyl) of estradiol were obtained from 3-O-benzyl-17.beta.-estradiol with sodium hydride/alkyl halide, followed by the removal of the O-benzyl protecting group via catalytic transfer hydrogenation. An increase compared to estradiol in the protection of neural (HT-22) cells against oxidative stress due to exposure of glutamate was furnished by higher (C-3 to C-8) alkyl ethers, while Me and Et ethers decreased the neuroprotective effect significantly. Lipophilic (Bu and octyl) ethers blocking the phenolic hydroxyl (3-OH) of A-ring were inactive.

ST alkoxyestratriene prepn neuroprotectant oxidative stress; estratriene alkoxy prepn neuroprotectant oxidative stress

IT Cytoprotective agents
(neuroprotectants; synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT Crystal structure
Molecular structure
Oxidative stress, biological
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT **319427-05-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT 4954-12-5P 21830-24-0P 128805-68-5P 319427-03-7P 319427-04-8P **319427-06-0P 319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT 50-28-2, 17.beta.-Estradiol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT 14982-15-1P 141318-37-8P 319426-98-7P 319426-99-8P 319427-00-4P 319427-01-5P 319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

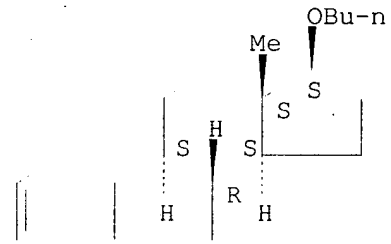
RE

(1) Anwer, M; Synthesis 1980, P929 HCAPLUS
(2) Behl, C; Biochem Biophys Res Commun 1995, V216, P473 HCAPLUS
(3) Behl, C; Cell 1994, V77, P817 HCAPLUS
(4) Behl, C; Mol Pharmacol 1997, V51, P535 HCAPLUS
(5) Bishop, J; Mol Cell Neurosci 1994, V5, P303 HCAPLUS
(6) Coombs, M; Steroids 1965, V6, P841 HCAPLUS
(7) Elamin, B; J Org Chem 1979, V44, P3442 HCAPLUS
(8) Ghose, A; J Comput Chem 1988, V9, P80 HCAPLUS
(9) Glenner, G; Cell 1988, V52, P307 HCAPLUS
(10) Green, P; J Neurocytol, in press
(11) Green, P; J Neurosci 1997, V17, P511 HCAPLUS

(12) Green, P; J Steroid Biochem Mol Biol 1997, V63, P229 HCAPLUS
(13) Green, P; Neurosci Lett 1996, V218, P165 HCAPLUS
(14) Green, P; Neuroscience 1998, V84, P7 HCAPLUS
(15) Gridley, K; Mol Pharmacol 1998, V54, P874 HCAPLUS
(16) Kawas, C; Neurology 1997, V48, P1517 HCAPLUS
(17) Maher, P; J Neurosci 1996, V15, P6394
(18) Mook-Jung, I; Neurosci Lett 1997, V235, P101 HCAPLUS
(19) Moorsmann, B; Proc Natl Acad Sci U S A 1999, V96, P8867
(20) Paganni-Hill, A; Am J Epidemiol 1994, V140, P256
(21) Pike, J; J Neurochem 1999, V72, P1552
(22) Qian, X; J Steroid Biochem 1988, V29, P657 HCAPLUS
(23) Sawada, H; J Neurosci Res 1998, V54, P707 HCAPLUS
(24) Shearman, M; Proc Natl Acad Sci U S A 1994, V91, P470
(25) Sheldrick, G; SHELXTL5 1998
(26) Yankner, B; Neuron 1996, V16, P921 HCAPLUS

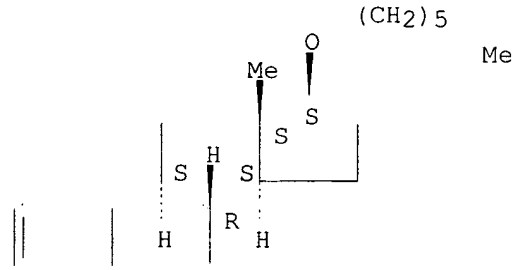
IT **319427-05-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RN 319427-05-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



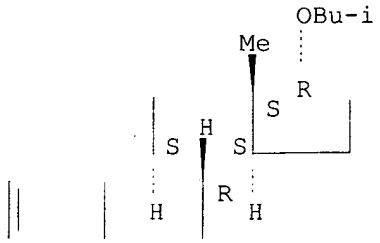
IT **319427-06-0P 319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RN 319427-06-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



(impurities detn. in, by HPLC)
IT **119309-39-6**, 17.alpha.-Isobutylestradiol
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in ethynylestradiol by HPLC)
RN 119309-39-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17.alpha.)- (9CI) (CA INDEX NAME)

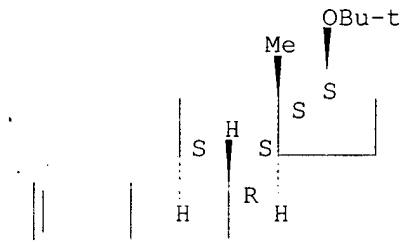
Absolute stereochemistry.



L27 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN 1976:554233 HCAPLUS
DN 85:154233
TI Study of the specificity of the estradiol-binding system of guinea pig uteri
AU Shchedrina, R. N.; Sturchak, S. V.; Bobrova, E. G.; Ishkov, V. L.; Pivnitskii, K. K.; Fanchenko, N. D.
CS All-Union Res. Inst. Obstet. Gynecol., Moscow, USSR
SO Byull. Eksp. Biol. Med. (1976), 82(8), 989-93
CODEN: BEBMAE
DT Journal
LA Russian
CC 2-3 (Hormone Pharmacology)
AB The affinities of 49 steroids for the estradiol [50-28-2]-binding system of guinea pig uteri were compared. The presence of free OH groups in positions 3 (phenol) and 17.beta. and reciprocal orientation were required for interaction with the receptor system. An intact steroid skeleton was not necessary. A polar function in ring C inhibited interaction. In addn. to estradiol, 17.alpha.-ethynylestradiol [57-63-6], synestrol, and diethylstilbestrol [56-53-1] had high affinities for the estradiol-binding system.
ST estradiol receptor interaction estrane deriv
IT Uterus, metabolism
(estradiol binding by, estrane derivs. in relation to)
IT Receptors
RL: BIOL (Biological study)
(for estradiol, of uterus, estrane derivs. interaction with)
IT Estrane, derivs.
RL: BIOL (Biological study)
(estradiol binding system of uterus interaction with)
IT 50-27-1 50-50-0 53-16-7 53-45-2 53-63-4 56-53-1 57-63-6
72-33-3 84-16-2 90-15-3 113-38-2 900-83-4 963-75-7 979-32-8
1035-77-4 1089-78-7 1125-78-6 1217-09-0 1624-62-0 1630-83-7
1852-96-6 2299-08-3 2529-64-8 2639-53-4 3736-22-9 6218-29-7
14550-57-3 15833-07-5 19590-55-7 32436-64-9 32436-65-0
32436-66-1 34124-99-7 **38781-59-8** 39662-38-9 40481-16-1
54064-57-2 54064-60-7 54064-61-8 58395-78-1 60779-03-5
60779-04-6 60779-05-7 60779-06-8 60788-62-7 60812-06-8
60827-74-9 60872-64-2
RL: BIOL (Biological study)

(estradiol binding system of uterus interaction with)
IT 50-28-2, biological studies
RL: BIOL (Biological study)
(uterus binding of)
IT **38781-59-8**
RL: BIOL (Biological study)
(estradiol binding system of uterus interaction with)
RN 38781-59-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

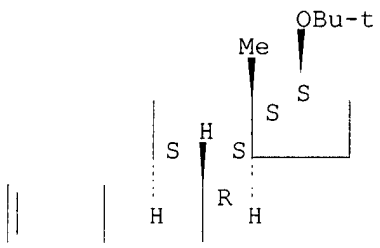
Absolute stereochemistry.



L27 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN 1974:121187 HCAPLUS
DN 80:121187
TI Replacing the phenol hydroxy group with hydrogen. Reductive cleavage of alkyl esters of estrogens by lithium in ethers
AU Cherkasov, A. N.; Golubovskaya, L. E.; Pivnitskii, K. K.
CS Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR
SO Zh. Org. Khim. (1974), 10(2), 320-8
CODEN: ZORKAE
DT Journal
LA Russian
CC 32-3 (Steroids)
GI For diagram(s), see printed CA Issue.
AB The estratrienol ether I (R = Me3CO) was refluxed in an Ar atm. in glyme contg. Li to give I (R = HO). Under the same conditions I (R = MeOCH2O, tetrahydro-2H-pyran-2-yloxy) yielded I (R = H), and I (R = MeO, Me2CHO) gave a mixt. of I (R = H, HO). Analogous cleavage products were obtained from estradiol and estrone ethers.
ST estratrienol ether cleavage; alkoxyestratriene ether cleavage
IT Steroids, reactions
RL: RCT (Reactant)
(3-alkoxy-1,3,5(10)-unsatd., reductive cleavage of)
IT 50-28-2, reactions
RL: RCT (Reactant)
(etherification of)
IT 53-16-7
RL: RCT (Reactant)
(ketalization and etherification of)
IT 38781-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 75-26-3 107-30-2
RL: RCT (Reactant)
(reaction of, with estratrienol)
IT 53-63-4
RL: RCT (Reactant)
(reaction of, with isopropylbromide)

IT 1852-96-6 3589-91-1 38781-54-3 **38781-59-8** 52509-95-2
52509-96-3 52509-97-4 52610-62-5
RL: RCT (Reactant)
(reductive cleavage of)
IT 115-11-7, reactions
RL: RCT (Reactant)
(with estratrienol)
IT **38781-59-8**
RL: RCT (Reactant)
(reductive cleavage of)
RN 38781-59-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17.beta.)- (9CI)
(CA INDEX NAME)

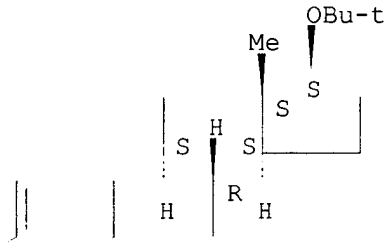
Absolute stereochemistry.



L27 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:501990 HCAPLUS
DN 77:101990
TI New method for the replacement of phenolic hydroxyl group by hydrogen. Reduction of alkoxyalkyl ethers of phenols by lithium
AU Cherkasov, A. N.; Pivnitskii, K. K.
CS Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR
SO Zh. Org. Khim. (1972), 8(1), 211-12
CODEN: ZORKAE
DT Journal
LA Russian
CC 32-3 (Steroids)
AB 3-(Methoxymethoxy)estrane and the tetrahydropyranyl ethers of estranol, estranediol, and estrone ethylene ketal were reduced by finely divided Li in refluxing MeOCH2CH2OMe to the corresponding 3-H compds. in 76-91% yield. The tert-Bu ethers of estranol and estranediol gave the corresponding phenols in 75-98% yields, resp., under identical conditions.
ST lithium redn steroidal phenol; alkoxyalkoxy steroid redn; dehydroxylation phenol steroidal
IT Steroids, reactions
RL: RCT (Reactant)
((alkoxyalkoxy), dealkoxylation of by lithium)
IT Dealkoxylation
(of (alkoxyalkoxy) steroids, by lithium)
IT 1217-09-0P 38781-61-2P 38781-62-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 53-63-4 1852-96-6 3589-91-1 14550-57-3 38781-53-2 38781-54-3
38781-56-5 38781-57-6 **38781-59-8**
RL: RCT (Reactant)
(reaction of, with lithium)
IT 7439-93-2, reactions
RL: RCT (Reactant)
(with (alkoxyalkoxy)estrane derivs.)

IT **38781-59-8**
RL: RCT (Reactant)
(reaction of, with lithium)
RN 38781-59-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



=> fil reg
FILE 'REGISTRY' ENTERED AT 11:38:55 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 27 MAY 2002 HIGHEST RN 422267-53-6
DICTIONARY FILE UPDATES: 27 MAY 2002 HIGHEST RN 422267-53-6

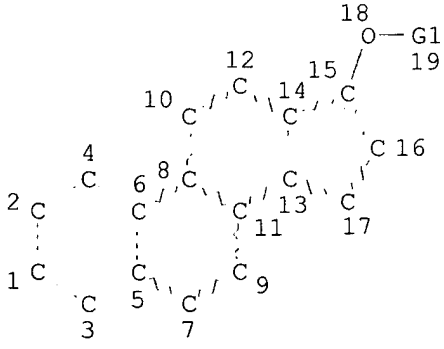
TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d sta que l32
L30 STR



VAR G1=AK/CB
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM

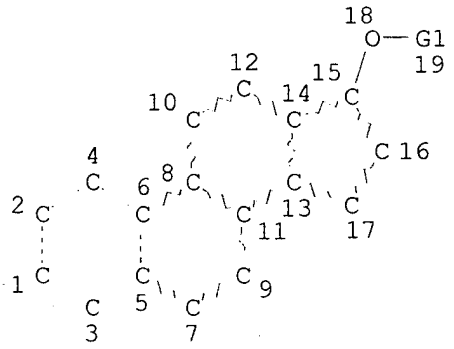
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 5
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L32 4506 SEA FILE=REGISTRY SSS FUL L30

100.0% PROCESSED 234011 ITERATIONS 4506 ANSWERS
SEARCH TIME: 00.00.21

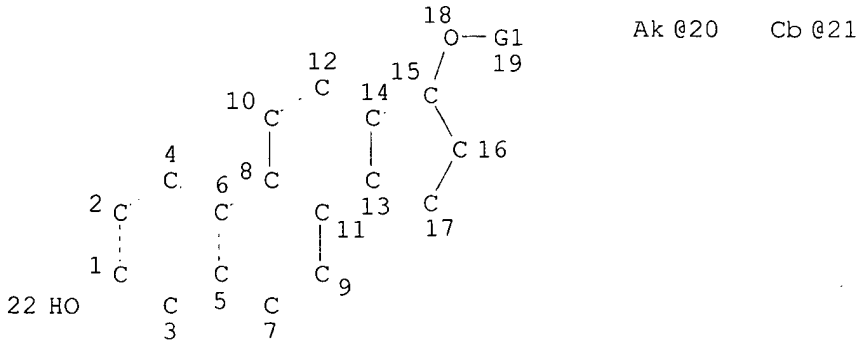
=> d sta que l51
L30 STR



VAR G1=AK/CB
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 5
NUMBER OF NODES IS 19

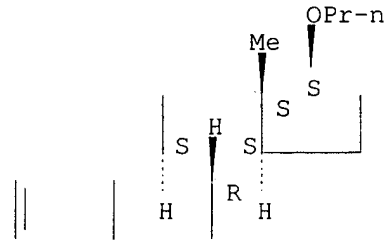
STEREO ATTRIBUTES: NONE
L32 4506 SEA FILE=REGISTRY SSS FUL L30
L49 STR



VAR G1=20/21
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 14
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M3 C AT 20
ECOUNT IS M3 C AT 21

```
GRAPH ATTRIBUTES:
RSPEC   5
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
L51          15 SEA FILE=REGISTRY SUB=L32 CSS FUL L49

100.0% PROCESSED   3944 ITERATIONS                          15 ANSWERS
SEARCH TIME: 00.00.01


=> d his

     (FILE 'REGISTRY' ENTERED AT 11:09:26 ON 29 MAY 2002)
                DEL HIS

     FILE 'HCAPLUS' ENTERED AT 11:09:34 ON 29 MAY 2002
                E PROKAI L/AU
L1           89 S E3,E4
L2            1 S E7
                E SIMPKINS J/AU
L3          227 S E3,E5,E7-E9
L4           22 S L1-L3 AND STERO?/SC,SX,CW
L5          123 S L1-L3 AND (?ESTROGEN? OR ?ESTRADIOL? OR ?STEROID?)
L6          126 S L4,L5
L7            8 S L1,L2 AND L3
L8            3 S L7 AND L4-L6
L9            0 S L6 AND ALKYLETHER
L10           2 S L6 AND ALKYL(L)ETHER
L11           2 S L10 AND L1-L10
                SEL RN

     FILE 'REGISTRY' ENTERED AT 11:12:06 ON 29 MAY 2002
L12          18 S E1-E18
L13          16 S L12 AND NR>=4
L14           5 S L13 AND (C22H32O2 OR C24H36O2 OR C26H40O2)
L15           3 S L14 NOT 3()(BUTOXY OR OCTYLOXY)
L16         777 S (C22H32O2 OR C24H36O2 OR C26H40O2)/MF AND C5-C6-C6-C6/ES
L17         110 S L16 AND 4432.3.65/RID AND 4/NR
L18         104 S L17 NOT 3 OL
L19           6 S L17 NOT L18
L20           5 S L19 NOT 13C#
L21           5 S L15,L20
                SEL RN
L22           0 S E19-E23/CRN

     FILE 'HCAOLD' ENTERED AT 11:20:06 ON 29 MAY 2002
L23           0 S L21

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:20:07 ON 29 MAY 2002
L24           1 S L21

     FILE 'HCAPLUS' ENTERED AT 11:20:18 ON 29 MAY 2002
L25           8 S L21
L26           3 S L1-L3 AND L25
L27           8 S L25,L26

     FILE 'REGISTRY' ENTERED AT 11:20:53 ON 29 MAY 2002

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:21:06 ON 29 MAY 2002
```

```
     FILE 'HCAPLUS' ENTERED AT 11:21:16 ON 29 MAY 2002

     FILE 'REGISTRY' ENTERED AT 11:21:39 ON 29 MAY 2002
L28             STR
L29           0 S L28 SAM
L30             STR L28
L31          21 S L30 SAM
L32        4506 S L30 FUL
               SAV TEMP L32 QAZI893324/A
L33        3917 S L32 AND 4432.3.65/RID
L34         589 S L32 NOT L33
L35             STR L28
L36           5 S L35 CSS SAM SUB=L32
L37         642 S L32 NOT ESTRA?
L38         314 S L37 NOT ?PREGN?/CNS
L39          86 S L38 NOT GONA?
L40          48 S L39 NOT CHOL?
L41        3864 S L32 NOT L37-L40
L42           3 S L32 NOT CN/FA
L43           5 S L35 CSS SAM SUB=L41
L44         100 S L35 CSS FUL SUB=L41
               SAV TEMP L44 QAZI893324A/A
L45          95 S L44 NOT L21
L46          93 S L45 NOT (ION OR LABELED OR (D OR T)/ELS OR 11C# OR 13C# OR 14
L47          22 S L46 AND 4/NR
L48           3 S L47 AND (C21H28O2 OR C21H26O2 OR C21H30O2)
L49             STR L35
L50           0 S L49 CSS SAM SUB=L32
L51          15 S L49 CSS FUL SUB=L32
               SAV L51 TEMP QAZI893324B/A
L52          13 S L51 NOT (13C# OR T/ELS)
L53           8 S L48,L52 NOT L21

     FILE 'HCAOLD' ENTERED AT 11:38:33 ON 29 MAY 2002
L54           0 S L53

     FILE 'HCAPLUS' ENTERED AT 11:38:36 ON 29 MAY 2002
L55          10 S L53

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:38:41 ON 29 MAY 2002
L56           1 S L53

     FILE 'REGISTRY' ENTERED AT 11:38:55 ON 29 MAY 2002

=> d ide can tot l53

L53  ANSWER 1 OF 8  REGISTRY  COPYRIGHT 2002 ACS
RN   319427-04-8  REGISTRY
CN   Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17.beta.)- (9CI)  (CA INDEX
     NAME)
FS   STEREOSEARCH
MF   C21 H30 O2
SR   CA
LC   STN Files:   CA, CAPLUS, USPATFULL

Absolute stereochemistry.
```



HO

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

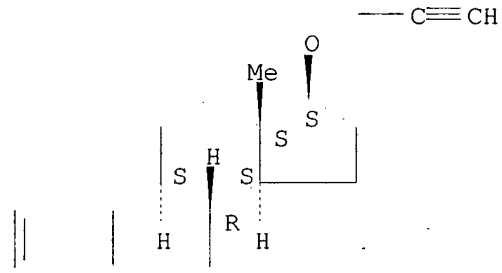
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L53 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 126003-44-9 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C21 H26 O2**
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Absolute stereochemistry.



HO

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

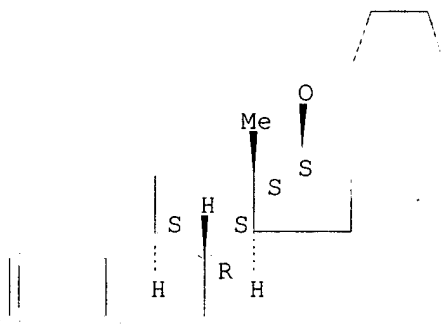
REFERENCE 1: 117:8261

REFERENCE 2: 112:158724

L53 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 85391-72-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(cyclopentyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

MF C23 H32 O2
SR Commission of European Communities
LC STN Files: CA, CAPLUS, CHEMLIST
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



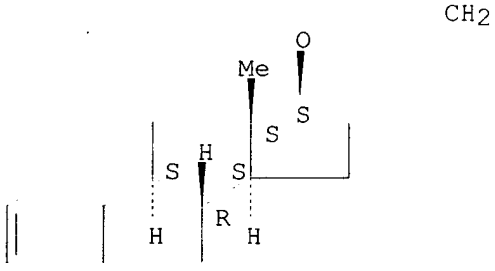
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 100:22887

L53 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 55561-41-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C21 H28 O2**
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

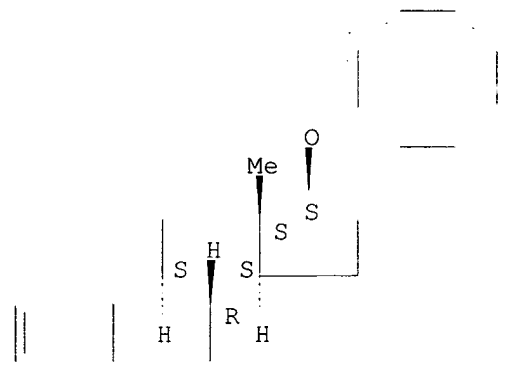
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:90134

REFERENCE 2: 82:125520

L53 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 41622-69-9 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cycloocten-1-yloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17.beta.-(Cyclooct-1'-enyloxy)estra-1,3,5(10)-trien-3-ol
FS STEREOSEARCH
MF C26 H36 O2
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



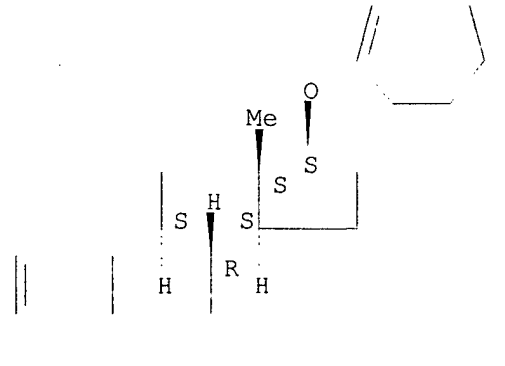
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:106316

L53 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 41622-66-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohepten-1-yloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H34 O2
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



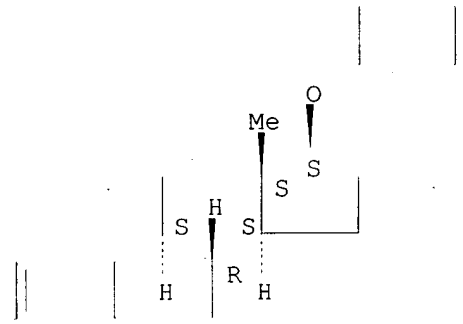
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:106316

L53 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 13885-34-2 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-3-ol, 17.beta.-(1-cyclohexen-1-yloxy)- (8CI)
FS STEREOSEARCH
MF C24 H32 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

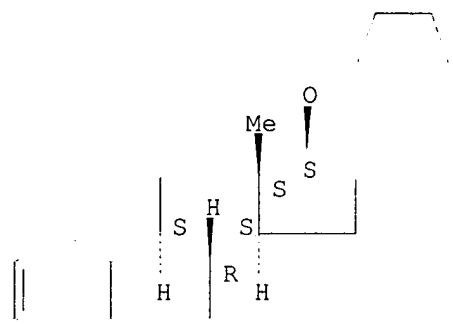
REFERENCE 1: 78:106316

REFERENCE 2: 70:68634

REFERENCE 3: 66:95293

L53 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 13885-30-8 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17.beta.-(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H30 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 70:68634

REFERENCE 2: 66:95293

=> fil uspatall
FILE 'USPATFULL' ENTERED AT 11:39:21 ON 29 MAY 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 11:39:21 ON 29 MAY 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

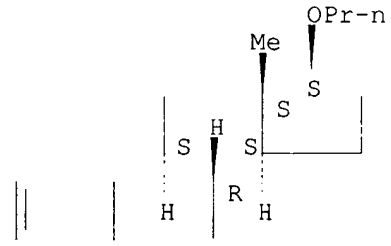
=> d bib abs hitstr l56

L56 ANSWER 1 OF 1 USPATFULL
AN 2002:61264 USPATFULL
TI Alkyl ether modified polycyclic compounds having a terminal phenol and uses for protection of cells
IN Prokai, Laszlo, Gainesville, FL, UNITED STATES
Simpkins, James W., Fort Worth, TX, UNITED STATES
PI US 2002035100 A1 20020321
AI US 2001-893324 A1 20010627 (9)
PRAI US 2000-214077P 20000627 (60)
DT Utility
FS APPLICATION
LREP BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618
CLMN Number of Claims: 46
ECL Exemplary Claim: 1
DRWN 5 Drawing Page(s)
LN.CNT 951
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Methods and compositions are provided for achieving a cytoprotective effect by selecting a polycyclic compound with a phenol group at one end of the molecule and a carbon ring at the other such that an alkyl ether functional group in which the alkyl group has a formula C.sub.nH.sub.2n+1 (where n is at least 3 and less than 20) is positioned on the carbon ring. The compound may be used to achieve a cytoprotective effect in cells and to retard the development of a degenerative condition in a subject suffering from a disease, trauma or aging.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **319427-04-8P**
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
RN 319427-04-8 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 11:39:34 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 29 May 2002 VOL 136 ISS 22
FILE LAST UPDATED: 27 May 2002 (20020527/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

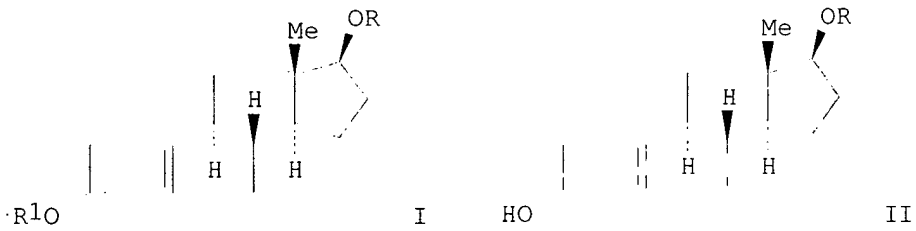
=> d l55 all hitstr tot

L55 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:10439 HCAPLUS
DN 136:85991
TI Preparation of 17.beta.-alkyl ether estradiol derivatives with cytoprotective activity of cells from degeneration through disease, trauma or aging
IN Prokai, Laszlo; Simpkins, James W.
PA University of Florida Research Foundation, Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2

DT Patent
LA English
IC ICM C07D
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000619	A2	20020103	WO 2001-US41170	20010627
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2002035100	A1	20020321	US 2001-893324	20010627
PRAI	US 2000-214077P	P	20000627		

GI



AB Cytoprotective compds. I (R = Me, Et, Pr, Bu, (CH2)5Me, or (CH2)7Me; R1 = OH) were prepd. in 50-75% yields from 17.beta.-estradiol. 17.beta.-Estradiol and benzyl halide in K2CO3 gave 93% yield of 3-benzyloxyestra-1,3,5(10)-trien-17.beta.-ol which was then alkylated with the appropriate alkyl halides in DMF and NaH yielding the 3-benzyloxy protected derivs. of I which were then deprotected via catalytic hydrogenation using ammonium formate in Pd/C. Thus compds. II (R = hexyl and octyl) were prepd. in 70 and 75% resp., and were neuroprotective to a similar extent at a concn. of 10 .mu.M and 1 .mu.M. Typical compns. contain approx. 0.01-95% by wt. of active ingredient and the percentage of active ingredient will depend upon the dosage form and mode of administration; an ED of the active agent as measured in the plasma of a subject may be in the range of 5pg/mL-5000pg/mL. Cytoprotective compds. I (R = OH; R1 = Bu, (CH2)7Me) were prepd. from 17.beta.-estradiol and Bu or octyl bromide in K2CO3 in 68 and 72% resp.

ST estradiol hydroxy alkylated deriv prepn cytoprotective compn; neuroprotective alkyl ether steroid prepn; crystal structure butoxyestratrienol

IT Steroids, preparation
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(alkylation of 17.beta.-OH or 3-OH; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Cytoprotective agents
(cardioprotective; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Nervous system

(degeneration; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Alkylation
(hydroxyalkylation; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Eye, disease
(macula, degeneration; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Crystal structure
(of 17.beta.-butoxyestra-1,3,5(10)-trien-3-ol)

IT Estrogen receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used as cytoprotective agents of cells from degeneration)

IT Anti-Alzheimer's agents
Anti-ischemic agents
Bone, disease
Drug delivery systems
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Osteoporosis
(therapeutic agents; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT 319427-05-9P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure)

IT 4954-12-5P 21830-24-0P 128805-68-5P 319427-03-7P
319427-04-8P 319427-06-0P 319427-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

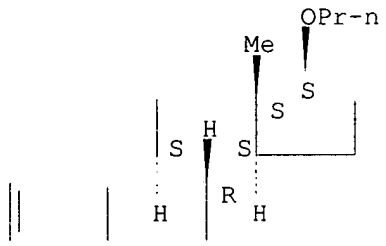
IT 50-28-2, 17.beta.-Estradiol, reactions 109-65-9, Butyl bromide 111-83-1, Octyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT 14982-15-1P 141318-37-8P 319426-98-7P 319426-99-8P 319427-00-4P 319427-01-5P 319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT **319427-04-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

RN 319427-04-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

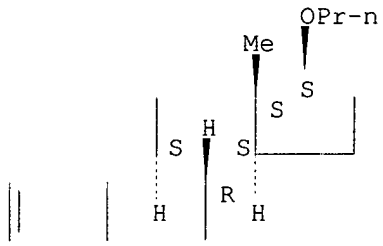
Absolute stereochemistry.



L55 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 2000:820327 HCAPLUS
DN 134:101056
TI Synthesis and Biological Evaluation of 17.beta.-Alkoxyestra-1,3,5(10)-trienes as Potential Neuroprotectants Against Oxidative Stress
AU Prokai, Laszlo; Oon, Su-Min; Prokai-Tatrai, Katalin; Abboud, Khalil A.; Simpkins, James W.
CS Center for Drug Discovery College of Pharmacy Department of Anesthesiology College of Medicine and Center for Neurobiology of Aging College of Pharmacy, University of Florida, Gainesville, FL, 32610-0497, USA
SO Journal of Medicinal Chemistry (2001), 44(1), 110-114
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
OS CASREACT 134:101056
AB 17.beta.-O-Alkyl ethers (Me, Et, Pr, Bu, hexyl, and octyl) of estradiol were obtained from 3-O-benzyl-17.beta.-estradiol with sodium hydride/alkyl halide, followed by the removal of the O-benzyl protecting group via catalytic transfer hydrogenation. An increase compared to estradiol in the protection of neural (HT-22) cells against oxidative stress due to exposure of glutamate was furnished by higher (C-3 to C-8) alkyl ethers, while Me and Et ethers decreased the neuroprotective effect significantly. Lipophilic (Bu and octyl) ethers blocking the phenolic hydroxyl (3-OH) of A-ring were inactive.
ST alkoxyestratriene prepn neuroprotectant oxidative stress; estratriene alkoxy prepn neuroprotectant oxidative stress
IT Cytoprotective agents
(neuroprotectants; synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT Crystal structure
Molecular structure
Oxidative stress, biological
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT 319427-05-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-

trienes as potential neuroprotectants against oxidative stress)
IT 4954-12-5P 21830-24-0P 128805-68-5P 319427-03-7P
319427-04-8P 319427-06-0P 319427-07-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT 50-28-2, 17.beta.-Estradiol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT 14982-15-1P 141318-37-8P 319426-98-7P 319426-99-8P 319427-00-4P
319427-01-5P 319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anwer, M; Synthesis 1980, P929 HCAPLUS
(2) Behl, C; Biochem Biophys Res Commun 1995, V216, P473 HCAPLUS
(3) Behl, C; Cell 1994, V77, P817 HCAPLUS
(4) Behl, C; Mol Pharmacol 1997, V51, P535 HCAPLUS
(5) Bishop, J; Mol Cell Neurosci 1994, V5, P303 HCAPLUS
(6) Coombs, M; Steroids 1965, V6, P841 HCAPLUS
(7) Elamin, B; J Org Chem 1979, V44, P3442 HCAPLUS
(8) Ghose, A; J Comput Chem 1988, V9, P80 HCAPLUS
(9) Glenner, G; Cell 1988, V52, P307 HCAPLUS
(10) Green, P; J Neurocytol, in press
(11) Green, P; J Neurosci 1997, V17, P511 HCAPLUS
(12) Green, P; J Steroid Biochem Mol Biol 1997, V63, P229 HCAPLUS
(13) Green, P; Neurosci Lett 1996, V218, P165 HCAPLUS
(14) Green, P; Neuroscience 1998, V84, P7 HCAPLUS
(15) Gridley, K; Mol Pharmacol 1998, V54, P874 HCAPLUS
(16) Kawas, C; Neurology 1997, V48, P1517 HCAPLUS
(17) Maher, P; J Neurosci 1996, V15, P6394
(18) Mook-Jung, I; Neurosci Lett 1997, V235, P101 HCAPLUS
(19) Moorsmann, B; Proc Natl Acad Sci U S A 1999, V96, P8867
(20) Paganni-Hill, A; Am J Epidemiol 1994, V140, P256
(21) Pike, J; J Neurochem 1999, V72, P1552
(22) Qian, X; J Steroid Biochem 1988, V29, P657 HCAPLUS
(23) Sawada, H; J Neurosci Res 1998, V54, P707 HCAPLUS
(24) Shearman, M; Proc Natl Acad Sci U S A 1994, V91, P470
(25) Sheldrick, G; SHELXTL5 1998
(26) Yankner, B; Neuron 1996, V16, P921 HCAPLUS
IT **319427-04-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RN 319427-04-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

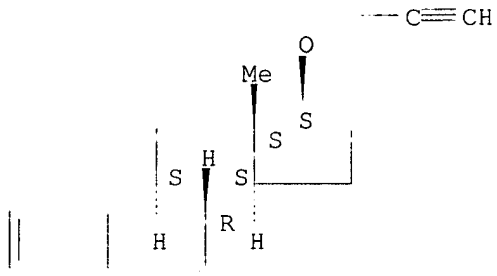


HO

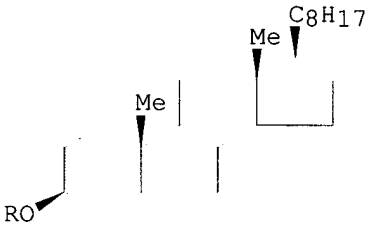
L55 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1992:408261 HCAPLUS
DN 117:8261
TI Synthesis of o-carboranylmethyl ethers of steroids as potential target substrates for boron neutron capture therapy
AU Schneiderova, Lenka; Strouf, Oldrich; Gruner, Bohumir; Pouzar, Vladimir; Drasar, Pavel; Hampl, Richard; Kimlova, Irena
CS Int. Inorg. Chem., Czech. Acad. Sci., Prague, 160 00, Czech.
SO Collect. Czech. Chem. Commun. (1992), 57(3), 463-71
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
CC 32-3 (Steroids)
AB o-Carboranylmethyl ethers of steroids were synthesized by insertion of steroidal 2-propynyloxy derivs. into 6,9-bis(acetonitrile)decaborane(12). This reaction afforded compds. with estrane and androstane skeleton, potentially useful in boron neutron capture therapy of hormone-sensitive forms of cancer, i.e., 17.beta.-o-carboranylmethyl ether of estradiol (I) (yield 14%) and 3.beta.- and 17.beta.-carboranylmethyl ethers of androstenediol (yield 12% and 13%, resp.). Jones oxidn. afforded carboranyl deriv. of androsten-17-one in 75% yield. As shown by a study of the insertion reaction of 3.beta.-(2-propynyloxy)cholest-5-ene, the low yields of the insertion reaction cannot be increased by changing the reaction conditions. The relative binding affinity of I to estrogen receptors from rat uterine and human breast tumor cytosol was 3.0 and 0.29% resp., of that of estradiol.
ST carboranylmethyl ether steroid; estrogen receptor binding carboranylmethoxyestrol
IT Receptors
RL: RCT (Reactant)
(estrogen, binding by, of estradiol carboranylmethyl ether)
IT Estrogens
RL: RCT (Reactant)
(receptors, binding by, of estradiol carboranylmethyl ether)
IT 141887-27-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and binding of, to estrogen receptors)
IT 141870-63-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn. of)
IT 138473-74-2P 141870-64-6P 141887-25-4P 141887-26-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 126003-29-0 126003-37-0 126003-41-6 **126003-44-9**
126003-45-0
RL: RCT (Reactant)
(reaction of, with carborane deriv.)
IT 17702-41-9, Decaborane(14) 28377-97-1 32124-79-1
RL: RCT (Reactant)

(reaction of, with hydroxy steroid)
IT **126003-44-9**
RL: RCT (Reactant)
(reaction of, with carborane deriv.)
RN 126003-44-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L55 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1990:158724 HCAPLUS
DN 112:158724
TI Steroids. Part CCCXLIII. Synthesis of 2-propynyl ethers of steroid alcohols
AU Pouzar, Vladimir; Schneiderova, Lenka; Drasar, Pavel; Strouf, Oldrich; Havel, Miroslav
CS Inst. Org. Chem. Biochem., Slovak Acad. Sci., Prague, 166 10/6, Czech.
SO Collect. Czech. Chem. Commun. (1989), 54(7), 1888-902
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
CC 32-7 (Steroids)
OS CASREACT 112:158724
GI

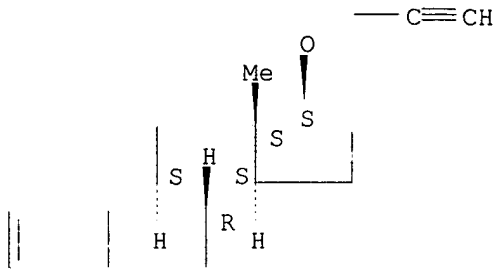


I

AB Title ethers were prepd. by treating the appropriate hydroxy steroid with CH.tplbond.CCH2Br under conditions of phase-transfer catalysis. Thus, cholesterol (I, R = H) was treated with CH.tplbond.CCH2Br under various phase-transfer conditions to give ether I (R = CH2C.tplbond.CH).
ST propynyl ether steroid alc
IT Etherification
(of hydroxy steroids with propargyl bromide under phase-transfer conditions)
IT Steroids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(propynyloxy, prepn. of, from propargyl bromide under phase-transfer

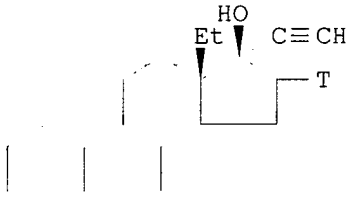
conditions)
IT 126003-46-1
RL: RCT (Reactant)
(Oppenauer oxidn. of)
IT 105644-82-4
RL: RCT (Reactant)
(detosylation-epimerization of)
IT 107-30-2
RL: RCT (Reactant)
(etherification by, of androstenediol acetate)
IT 106-96-7, Propargyl bromide
RL: RCT (Reactant)
(etherification by, of hydroxy steroids under phase-transfer conditions)
IT 1639-43-6
RL: RCT (Reactant)
(etherification of, with chloromethyl Me ether)
IT 53-43-0 57-88-5, Cholesterol, reactions 145-13-1 66168-96-5 88128-34-1
RL: RCT (Reactant)
(etherification of, with propargyl bromide under phase-transfer conditions)
IT 58-22-0
RL: RCT (Reactant)
(etherification of,, with propargyl bromide under phase-transfer conditions)
IT 126003-45-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and Oppenauer oxidn. of)
IT 126003-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deacetylation of)
IT 126003-33-6P 126003-36-9P 126003-39-2P 126003-43-8P 126003-47-2P 126024-80-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of)
IT 41781-86-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and etherification of, with propargyl bromide)
IT 5419-51-2P 126003-32-5P 126003-38-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and etherification of, with propargyl bromide under phase-transfer conditions)
IT 4975-52-4P 18000-76-5P 126003-29-0P 126003-30-3P 126003-34-7P 126003-35-8P 126003-37-0P 126003-40-5P 126003-41-6P 126003-42-7P **126003-44-9P** 126003-48-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 110-87-2
RL: RCT (Reactant)
(O-protection by, of hydroxysteroids)
IT 53-16-7, reactions
RL: RCT (Reactant)
(O-protection of, with dihydropyran)
IT **126003-44-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 126003-44-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

L55 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1984:22887 HCAPLUS
DN 100:22887
TI Tritium NMR spectroscopy of steroids
AU Funke, Carel W.; Kasperen, Frans M.; Wallaart, Jan; Wagenaars, Gerard N.
CS Sci. Dev. Group, Organon, Oss, 5340 BH, Neth.
SO J. Labelled Compd. Radiopharm. (1983), 20(7), 843-53
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
CC 32-5 (Steroids)
Section cross-reference(s): 22
GI

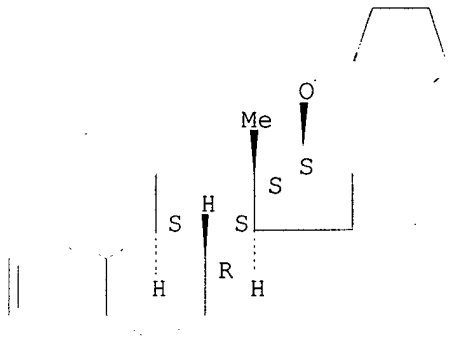


O I

AB Seven tritiated pregnane-type steroids, e.g. I, were prepd. and their T NMR spectra were studied; these spectra gave quant. information on the T distribution in these compds.
ST tritium NMR steroid
IT Nuclear magnetic resonance
(of tritium, in pregnanes)
IT Steroids, properties
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydroxy, tritium-labeled, prepn. and NMR of)
IT **85391-72-6**
RL: RCT (Reactant)
(exchange reaction of, with tritium)
IT 88247-77-2P 88247-78-3P 88247-79-4P 88247-80-7P 88255-64-5P
88255-65-6P 88255-66-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR of)
IT 73991-16-9 88247-81-8
RL: RCT (Reactant)
(redn.-tritiation of)
IT 54024-21-4
RL: RCT (Reactant)
(tritiation and ethynylation of)
IT 87863-63-6 88247-82-9 88247-84-1

RL: RCT (Reactant)
(tritiation, ethynylation, and hydrolysis of)
IT **85391-72-6**
RL: RCT (Reactant)
(exchange reaction of, with tritium)
RN 85391-72-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(cyclopentyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

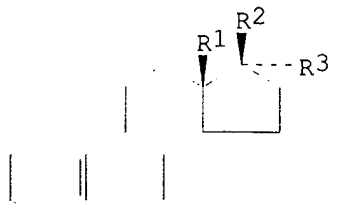
Absolute stereochemistry.



L55 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1977:90134 HCAPLUS
DN 86:90134
TI Esterification of phenolic hydroxyl groups in steroids
IN Schwarz, Sigfrid; Weber, Gisela
PA E. Ger.
SO Ger. (East), 5 pp. Addn. to Ger.(East) 114,806.
CODEN: GEXXA8
DT Patent
LA German
IC C07C167-28
CC 32-3 (Steroids)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DD 120016	Y	19760520	DD 1975-184239	19750217

GI



I

AB Estratrienyl sulfonates I [R = R4SO2, (R4 = Me2CH, PhCH2, Me(CH2)7, 4-MeC6H4, cyclopentyl, cyclohexyl); R1 = H, Me, R2R3 = O, MeON; R2 = HO, MeO, Me3SiO, BuCO2, EtCO2, PhCH2CH2CO2, CH2:CHCH2O; R2 = H, HC.tplbond.C, ClC.tplbond.C, CH2:CH] (20 compds.) were prepd. in 76-97% yields by treatment of I (R = H) in H2O contg. an alkali hydroxide or an alk. earth hydroxide and a quaternary ammonium salt with R4SO2Cl. Thus, I (R = R1 =

H, R2 = OH, R3 = C.tplbond.CH) in H2O-NaOH contg. (PhCH2)4N+Cl- was treated with Me2CHSO2Cl to give 80% I (R = Me2CHSO2, R1 = H, R2 = OH, R3 = C.tplbond.CH).

ST alkanesulfonate estratrienyl; sulfonation norpregnenynol; ethynylestradiol sulfonation; estradiol sulfonation; estrone sulfonation

IT 19-Norsteroids
RL: RCT (Reactant)
(3.beta.-hydroxy-17-oxygenated-1,3,5(10)-unsatd., sulfonates)

IT 28913-23-7P 28913-25-9P 29017-43-4P 29017-44-5P 29017-45-6P
32162-69-9P 38022-64-9P 38022-65-0P 42738-04-5P 42738-09-0P
42738-11-4P 54983-35-6P 55561-16-5P 55561-21-2P 55561-22-3P
55561-24-5P 55561-25-6P 55561-29-0P 55561-31-4P 61872-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 1939-99-7 4837-38-1 7795-95-1 10147-37-2 26394-17-2
RL: RCT (Reactant)
(reaction of, with estradienol)

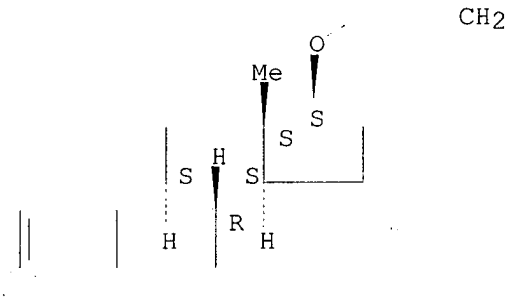
IT 50-28-2, reactions 53-16-7, reactions 57-63-6 3342-64-1 3758-34-7
4567-67-3 4954-12-5 7678-95-7 14012-72-7 26443-03-8 28416-77-5
33526-46-4 33760-44-0 42737-82-6 **55561-41-6**
RL: RCT (Reactant)
(sulfonylation of)

IT **55561-41-6**
RL: RCT (Reactant)
(sulfonylation of)

RN 55561-41-6 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L55 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2002 ACS

AN 1975:125520 HCAPLUS

DN 82:125520

TI Steroids. 15. Sulfonyloxy derivatives of estrogens

AU Schwarz, S.; Weber, G.; Schreiber, M.

CS Wiss. Lab., VEB Jenapharm, Jena, E. Ger.

SO Pharmazie (1975), 30(1), 17-21
CODEN: PHARAT

DT Journal

LA German

CC 32-5 (Steroids)

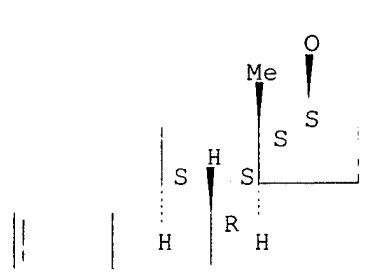
GI For diagram(s), see printed CA Issue.

AB Estranes I (R = alkyl, cycloalkyl, CH2Ph, aminoalkyl; R1 = C.tplbond.CH, C.tplbond.CCl, CH:CH2, Et, H; R2 = OH, OSiMe3, alkoxy, acyloxy; R1R2 = O, NOH, NOSiMe3, NOAc, NOMe) (66 compds.) were prepd., e.g. by treating the 3-hydroxyestranes with RSO2Cl.

ST estrane sulfonyloxy; sulfonate estrane; norpregnatrienyl alkanesulfonate; estradiol alkanesulfonate; ethynylestradiol alkanesulfonate

IT 19-Norsteroids
RL: RCT (Reactant)
(3-hydroxy-1,3,5(10)-unsatd., sulfonated)
IT 41781-86-6
RL: RCT (Reactant)
(alkylation of)
IT 57-63-6
RL: RCT (Reactant)
(esterification of)
IT 1689-02-7 1828-66-6 10147-37-2 10539-95-4 13360-57-1 20588-68-5
26394-17-2 35856-62-3
RL: RCT (Reactant)
(esterification of 17-(trimethylsiloxy)-19-nor-17.alpha.-pregna-
1,3,5(10)-trien-20-yn-3-ol by)
IT 10147-37-2
RL: RCT (Reactant)
(esterification of norpregnatrienynediol)
IT 28416-77-5
RL: RCT (Reactant)
(esterification of, with sulfonyl chlorides)
IT 4954-12-5P **55561-41-6P** 55561-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)
IT 55561-43-8P 55561-44-9P 55561-45-0P 55561-46-1P 55561-47-2P
55561-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and etherification of)
IT 55561-38-1P 55561-39-2P 55561-40-5P 55561-49-4P 55561-50-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
IT 3381-23-5P 28913-31-7P 28913-32-8P 28913-34-0P 28913-44-2P
29017-43-4P 29017-44-5P 42738-04-5P 42738-09-0P 42738-11-4P
52310-88-0P 52310-89-1P 52310-90-4P 54983-32-3P 54983-33-4P
55561-09-6P 55561-10-9P 55561-11-0P 55561-12-1P 55561-13-2P
55561-14-3P 55561-16-5P 55612-89-0P 55786-15-7P 55786-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)
IT 4236-42-4P 28913-23-7P 28913-35-1P 28913-36-2P 54983-34-5P
54983-35-6P 54983-36-7P 54983-37-8P 54983-38-9P 55561-15-4P
55561-17-6P 55561-18-7P 55561-19-8P 55561-20-1P 55561-21-2P
55561-23-4P 55561-24-5P 55561-25-6P 55561-26-7P 55561-27-8P
55561-28-9P 55561-29-0P 55561-30-3P 55561-31-4P 55561-32-5P
55561-33-6P 55561-34-7P 55561-35-8P 55561-36-9P 55561-37-0P
55561-51-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 55561-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., esterification, and etherification of)
IT **55561-41-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)
RN 55561-41-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17.beta.)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



HO

L55 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1973:106316 HCAPLUS
DN 78:106316
TI 1,3,5(10)-Estratrien-17.beta.-yl enol ethers and acetals. New classes of orally and parenterally active estrogenic derivatives
AU Gardi, Rinaldo; Vitali, Romano; Falconi, Giovanni; Ercoli, Alberto
CS Warner Vistor Steroid Res. Inst., Casatenovo, Italy
SO J. Med. Chem. (1973), 16(2), 123-7
CODEN: JMCMAR
DT Journal
LA English
CC 2-5 (Hormone Pharmacology)
AB A no. of labile 17-ethers of estradiol showed uterotrophic activity greater than that of estradiol, and in some cases comparable to that of ethynylestradiol. Esp. active orally at 0.3-0.9 nmole/day in mice were cycloalkenyl ethers with 5-9-membered rings, such as 17.beta.-(cyclopent-1-enyloxy)estra-1,3,5(10)-trien-3-ol propionate (I) [13885-28-4], and mixed ketals such as 17.beta.-[(1-methoxycyclopentyl)oxy]estra-1,3,5(10)-trien-3-ol (II) [13885-25-1]. High and long-lasting parenteral uterotrophic activity in rats was shown after single s.c. doses of 0.05 .mu.mole of cycloalkenyl ethers with 8-15-membered rings such as 17.beta.-(cyclooct-1-enyloxy)estra-1,3,5(10)-trien-3-ol m-chlorobenzoate [28275-58-3]. The depot activity of these compds. may result from their high lipophilicity and from slow cleavage of the ether linkage to release estradiol. The enol ethers were prepd. from the parent 17.beta.-hydroxyestratrienes by acid-catalyzed exchange etherification with alkyl enol ethers or acetals of the appropriate aldehyde or ketone. The acetal and ketal derivs. were prepd. by acid-catalyzed addn. of the 17.beta.-hydroxy steroid to suitable Me or Et enol ethers.
ST estradiol enol ether estrogen; uterotrophic estradiol enol ether
IT Estrogenic hormones
RL: BIOL (Biological study)
(estratrienyl acetals and enol ethers)
IT Uterus
(estratrienyl acetals and enol ethers effect on)
IT Molecular structure-biological activity relationship
(estrogenic, of estratrienyl acetals and enol ethers)
IT 53-16-7
RL: RCT (Reactant)
(acylation of)
IT 3000-64-4P 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P
13885-29-5P 13885-31-9P 13885-32-0P **13885-34-2P**
13885-35-3P 13885-36-4P 13945-91-0P 13945-92-1P 21513-21-3P
28151-76-0P 28151-78-2P 28151-79-3P 28151-80-6P 28200-87-5P
28200-89-7P 28200-91-1P 28200-93-3P 28200-94-4P 28200-96-6P
28200-97-7P 28200-99-9P 28201-00-5P 28201-01-6P 28201-02-7P
28201-03-8P 28201-04-9P 28201-05-0P 28231-33-6P 28275-57-2P
28275-58-3P 28275-59-4P 28275-62-9P 41622-58-6P 41622-59-7P

41622-60-0P 41622-64-4P 41622-65-5P **41622-66-6P**
41622-69-9P 41622-83-7P 41622-84-8P 41622-92-8P
41622-93-9P 41622-94-0P 41622-95-1P 41622-96-2P 41622-97-3P
41622-98-4P 41622-99-5P 41623-00-1P 41623-01-2P 41623-02-3P
41623-03-4P 41623-04-5P 41623-05-6P 41623-06-7P 41623-09-0P
41623-10-3P 41623-11-4P 41623-12-5P 41623-16-9P 41623-20-5P
41623-21-6P 41680-40-4P 41787-78-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and estrogenic activity of)

IT 28151-74-8P 28151-75-9P 28151-77-1P 28200-88-6P 28275-51-6P
28275-52-7P 28275-53-8P 28275-54-9P 28275-55-0P 28275-56-1P
41623-22-7P 41623-27-2P 41623-29-4P 41623-30-7P 41623-35-2P
41623-37-4P 41623-41-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

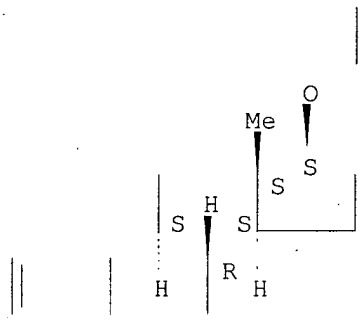
IT 502-72-7 931-57-7 41623-39-6
RL: BIOL (Biological study)
(reaction with estradiol esters)

IT 957-17-5
RL: BIOL (Biological study)
(reaction with estrones)

IT **13885-34-2P 41622-66-6P 41622-69-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and estrogenic activity of)

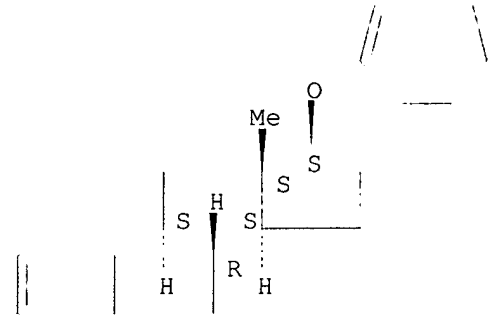
RN 13885-34-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 41622-66-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohepten-1-yloxy)-, (17.beta.)- (9CI)
(CA INDEX NAME)

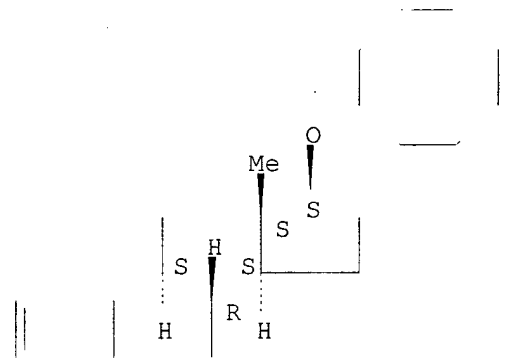
Absolute stereochemistry.



HO

RN 41622-69-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cycloocten-1-yloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



HO

L55 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1969:68634 HCAPLUS
DN 70:68634
TI 17-Ethers of estradiol
IN Ercoli, Alberto; Gardi, Rinaldo
PA Warner-Lambert Pharmaceutical Co.
SO U.S., 5 pp.
CODEN: USXXAM
DT Patent
LA English
NCL 424243000
CC 32 (Steroids)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3417183	A	19681217	US 1966-546506	19660502
	CH 479568	A	19691015	CH 1966-479568	19660601
	CH 483410	A	19691231	CH 1966-483410	19660601
	DK 118462	B	19700824	DK 1966-2868	19660603
	DK 121437	B	19711018	DK 1969-3171	19690612
PRAI	IT 1965-12593		19650604		

GI For diagram(s), see printed CA Issue.
AB The title compds. (I) are prepd. by treating a 3-ester of estradiol with a

functional deriv. of a carbonyl compd. in the presence of a catalyst. Thus, a soln. of 1 g. estradiol 3-propionate (II) in 2 ml. tert-BuOH is treated with 1 ml. cyclopentanone enol methyl ether and 10 mg. p-MeC6H4SO3H to give the 17-(1-methoxycyclopentyl) (A) ether of II, m. 81-3.degree. (MeOH-CH2Cl2), [.alpha.]2D2 44.5.degree. (c 0.5, dioxane). Similarly is prepd. the A ether of estradiol 3-acetate (III), m. 89-91.degree., [.alpha.]2D2 49.5.degree. (c 0.5%, dioxane). A soln. of 0.5 g. III in 25 ml. MeOH is refluxed 2 hrs. with 0.1N NaOH, the mixt. concd., and the residue crystd. from MeOH- CH2Cl2 to give the A ether of estradiol, m. 127-9.degree., [.alpha.]2D2 50.degree. (c = 0.5, dioxane). Similarly are prepd. the following I [R, R1, m.p., and [.alpha.]2D2 (c 0.5, dioxane) given]: EtCO, 1-methoxycyclohexyl, -, 49.degree.; Ac, 1-methoxycyclohexyl, 79-82.degree., 51.5.degree.; H, 1-methoxycyclohexyl, 108-10.degree., 53.5.degree.; EtCO, MeOC(Me)Et, 53-7.degree., 64.degree.; H, MeOC(Me)Et, 109-13.degree., 67.5.degree.. A mixt. of 3 g. II and 5 ml. cyclopentanone diethyl acetal is heated 1 hr. at 180-200.degree., neutralized with a few drops pyridine, concd. to dryness in vacuo, and crystd. from MeOH to give the 17-(cyclopent-1-enyl) ether of II, m. 91-3.degree., [.alpha.]2D2 61.5.degree. (c 0.5, dioxane). Similarly are obtained the following I [R, R1, m.p., [.alpha.]2D2 (c 0.5, dioxane) given]: Ac, cyclopent-1-enyl, 126-8.degree., 65.degree.; BuCO, cyclopent-1-enyl, - (oil), 53.5.degree.; H, cyclopent-1-enyl, 73-6.degree., 66.5.degree.; EtCO, cyclohex-1-enyl, 94-6.degree., 71.degree.; Ac, cyclohex-1-enyl, 114-16.degree., 75.degree.; BuCO, cyclohex-1-enyl, - (oil), 62.5.degree.; H, cyclohex-1-enyl, 87-90.degree., 75.5.degree.. I possess valuable claudogenic and estrogenic activity, esp. suitable for oral use. It is advisable to stabilize the pharmaceutical compns. with alk. substances to prevent acid hydrolysis of the 17-ethers.

ST estradiols estrogenic; estrogenic estradiols

IT 19-Norsteroids
RL: RCT (Reactant)
(alkoxy)

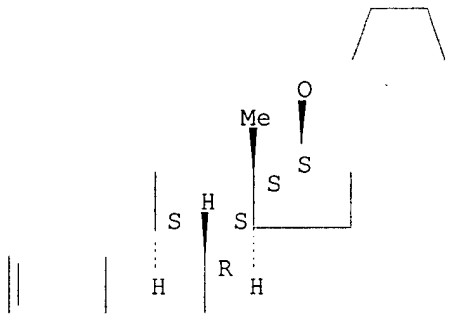
IT 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P 13885-29-5P
13885-30-8P 13885-31-9P 13885-32-0P 13885-33-1P
13885-34-2P 13885-35-3P 13885-36-4P 13885-37-5P
13945-91-0P 13945-92-1P 14258-73-2P 21513-21-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **13885-30-8P 13885-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 13885-30-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17.beta.-(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)

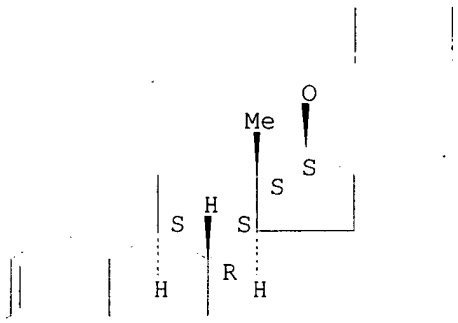
Absolute stereochemistry.



HO

RN 13885-34-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L55 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2002 ACS
AN 1967:95293 HCAPLUS
DN 66:95293
TI Estradiol ethers
PA Vismara, Francesco Societa per Azioni
SO Neth. Appl., 10 pp.
CODEN: NAXXAN
DT Patent
LA Dutch
IC C07C
CC 32 (Steroids)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI NL 6607527		19661205		
PRAI IT		19650604		

AB Estradiol 3-propionate (I) (1 g.) in 2 cc. tert-BuOH and 1 cc. cyclopentanone enol Me ether treated about 10 min. with 10 mg. p-MeC6H4SO3H yielded the 17-(1-methoxycyclopentyl) ether (II) of I, m. 81-3.degree. (CH2Cl2-MeOH), [.alpha.]22D 44.5.degree. (c 0.5, dioxane). Similarly was prepd. the 17-(1-methoxycyclopentyl) ether of estradiol 3-acetate (III), m. 89-91.degree., [.alpha.]22D 49.5.degree. (c 0.5, dioxane). II (0.5 g.) in 25 cc. MeOH refluxed 2 hrs. with 0.1N NaOH gave the 17-(1-methoxycyclopentyl) ether of estradiol (IV), m. 127-9.degree. [(CH2Cl)2-MeOH]. I (1 g.) in 2 cc. tert-BuOH and 1 cc. cyclohexanone enol Me ether treated with 10 mg. p-MeC6H4SO3H.C5H5N (V) gave the 17-(1-methoxycyclohexyl) ether (VI) of I. Similarly was prepd. 0.95 g. 17-(1-methoxycyclohexyl) ether of III, m. 79-82.degree., [.alpha.]22D 51.5.degree. (c 0.5, dioxane), from 1 g. III; its hydrolysis with 0.1N KOH gave the 17-(1-methoxycyclohexyl) ether of IV, m. 108-10.degree., [.alpha.]22D 53.5.degree. (c 0.5, dioxane). I (3 g.) and 5 cc. cyclopentanone dimethyl acetal heated 1 hr. at 180-200.degree. gave the 17-(1-cyclopentenyl) ether (VII) of I, m. 91-3.degree. (MeOH), [.alpha.]22D 61.5.degree. (c 0.5, dioxane). Similarly were prepd. the 17-(1-cyclopentenyl) ether of III, m. 126-8.degree., [.alpha.]22D 65.degree. (c 0.5, dioxane), and the oily 17-(1-cyclopentenyl) ether of estradiol 3-valerate (VIII), [.alpha.]22D 53.5.degree. (c 0.5, dioxane) VII (1.5 g.) in 50 cc. MeOH warmed 2 hrs. with 0.5 g. K2CO3 in 5 cc. H2O yielded the 17-(1-cyclopentenyl) ether of IV, m. 73-6.degree., [.alpha.]22D 66.5.degree. (c 0.5, dioxane). I (2 g.), 3 cc. cyclohexanone

dimethyl acetal, 20 mg. V, and 3 cc. HCONMe2 heated 1 hr. at 180-90.degree. gave the 17-(1-cyclohexenyl) ether (IX) of I, m. 94-6.degree. (CH2Cl2-MeOH), [.alpha.]22D 71.degree. (c 0.5, dioxane). Similarly were prepd. the 17-(1-cyclohexenyl) ether of III, m. 114-16.degree., [.alpha.]22D 75.degree. (c 0.5, dioxane), and the oily 17-(1-cyclohexenyl) ether of VIII, [.alpha.]22D 62.5.degree. (c 0.5, dioxane). IX (2 g.) hydrolyzed with NaOH-MeOH gave the 17-(1-cyclohexenyl) ether of IV, m. 87-90.degree., [.alpha.]22D 75.5.degree. (c 0.5, dioxane). EtMeC(OMNe)2 (1 g.), 30 mg. p-MeC6H4SO3H, and 5 cc. tert-BuOH with 1 g. I gave the 17-(1-methoxy-1-methylpropyl) ether of I, m. 64-8.degree., [.alpha.]22D 62.degree. (c 0.5, dioxane). Similarly was prepd. the 17-(1-methoxy-1-methylpropyl) ether of III, m. 53-7.degree., [.alpha.]22D 64.degree. (c 0.5, dioxane), which hydrolyzed with alkali gave the 17-(1-methoxy-1-methylpropyl) ether of IV, m. 109-13.degree., [.alpha.]22D 67.5.degree. (c 0.5, dioxane).

ST ESTRADIOL CYCLOPENTYL ETHERS; CYCLOPENTYL ETHERS ESTRADIOL; ESTRADIOL CYCLOHEXYL ETHERS; CYCLOHEXYL ETHERS ESTRADIOL; ESTRADIOL CYCLOPENTENYL ETHERS; CYCLOPENTENYL ETHERS ESTRADIOL; ESTRADIOL CYCLOHEXENYL ETHERS; CYCLOHEXENYL ETHERS ESTRADIOL; ESTRADIOL PROPYL ETHERS

IT Steroids, preparation
RL: PREP (Preparation)
(17-alkoxy)

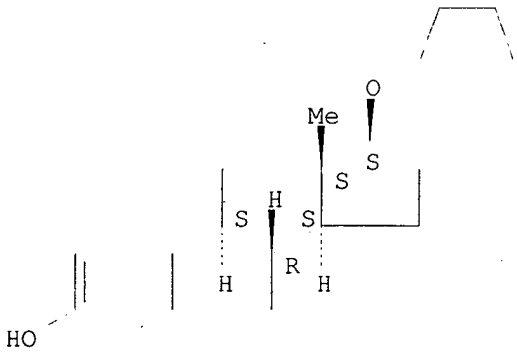
IT 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P 13885-29-5P
13885-30-8P 13885-31-9P 13885-32-0P 13885-33-1P
13885-34-2P 13885-35-3P 13885-36-4P 13885-37-5P
13945-91-0P 13945-92-1P 14258-73-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **13885-30-8P 13885-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 13885-30-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17.beta.-(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)

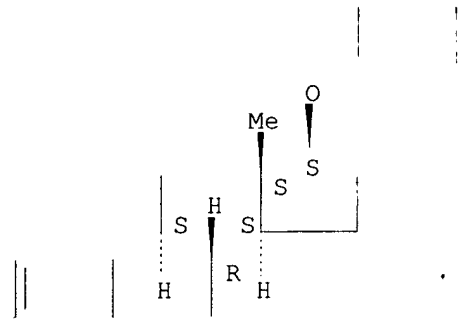
Absolute stereochemistry.



RN 13885-34-2 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

=> fil reg
FILE 'REGISTRY' ENTERED AT 11:45:42 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 27 MAY 2002 HIGHEST RN 422267-53-6
DICTIONARY FILE UPDATES: 27 MAY 2002 HIGHEST RN 422267-53-6

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

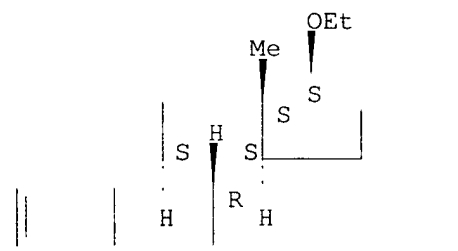
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d ide can tot l63

L63 ANSWER 1 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **319427-03-7** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.



HO

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

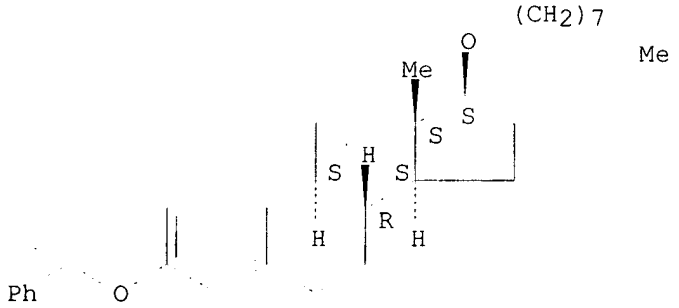
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L63 ANSWER 2 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **319427-02-6** REGISTRY
CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H46 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

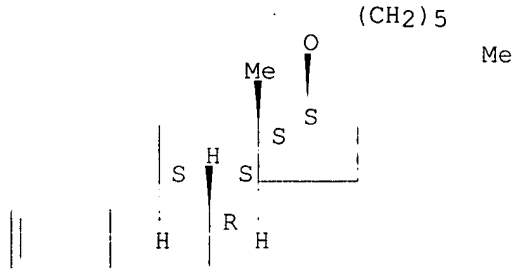
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L63 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **319427-01-5** REGISTRY
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H42 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



Ph O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

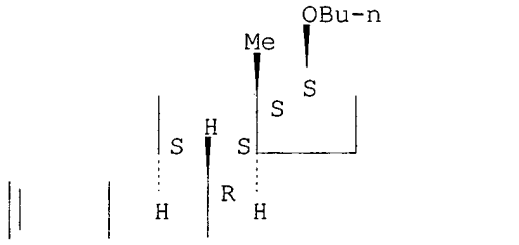
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L63 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **319427-00-4** REGISTRY
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H38 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



Ph O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

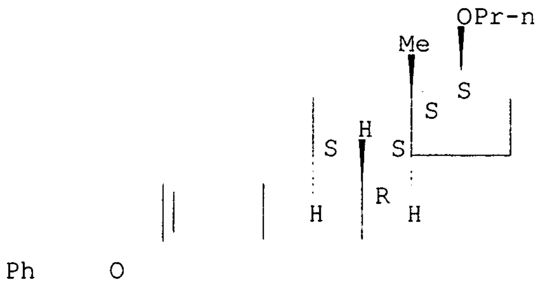
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L63 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **319426-99-8** REGISTRY
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H36 O2

SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

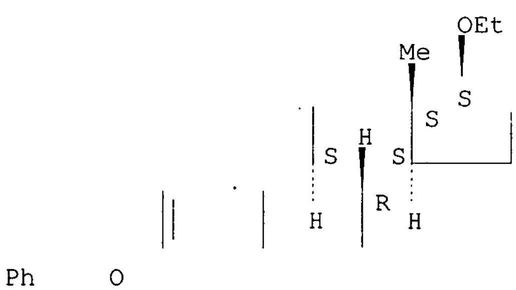
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE   1: 136:85991

REFERENCE   2: 134:101056

L63 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN   **319426-98-7** REGISTRY
CN   Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS   STEREOSEARCH
MF   C27 H34 O2
SR   CA
LC   STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

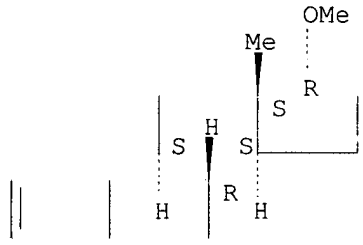
REFERENCE   1: 136:85991

REFERENCE   2: 134:101056

L63 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN   **182823-27-4** REGISTRY
CN   Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.alpha.)- (9CI) (CA INDEX

NAME)
FS STEREOSEARCH
MF C19 H26 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



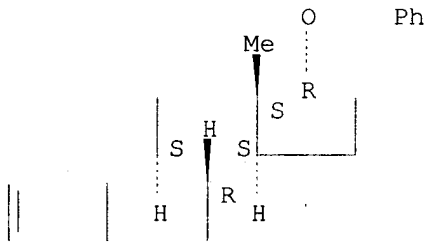
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:294029

L63 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **182624-51-7** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H30 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

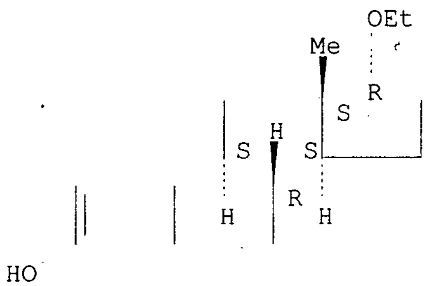
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:294029

L63 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **182624-49-3** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.alpha.)- (9CI) (CA INDEX

NAME)
FS STEREOSEARCH
MF C20 H28 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



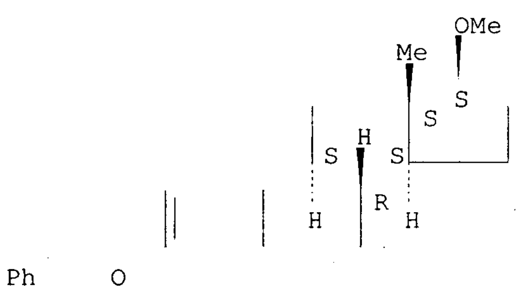
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:294029

L63 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **141318-37-8** REGISTRY
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H32 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

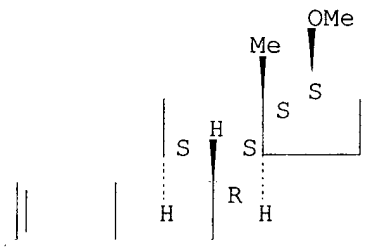
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 116:235946

L63 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2002 ACS
RN **4954-12-5** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-3-ol, 17.beta.-methoxy- (7CI, 8CI)
OTHER NAMES:
CN 17-Methoxy-1,3,5(10)-estratrien-3-ol
CN 17.beta.-Methoxyestra-1,3,5(10)-trien-3-ol
FS STEREOSEARCH
MF C19 H26 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
16 REFERENCES IN FILE CAPLUS (1967 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 130:293190

REFERENCE 4: 129:54482

REFERENCE 5: 116:235946

REFERENCE 6: 100:96847

REFERENCE 7: 89:2201

REFERENCE 8: 86:90134

REFERENCE 9: 82:125520

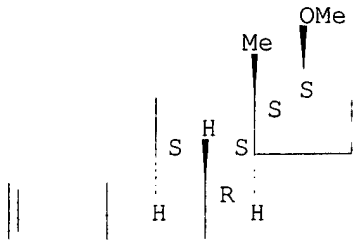
REFERENCE 10: 79:133109

=> d his l63-

(FILE 'REGISTRY' ENTERED AT 11:40:22 ON 29 MAY 2002)
L63 11 S L62 NOT (ACETATE OR 17 17 DIMETHOXY)

FILE 'HCAOLD' ENTERED AT 11:45:14 ON 29 MAY 2002

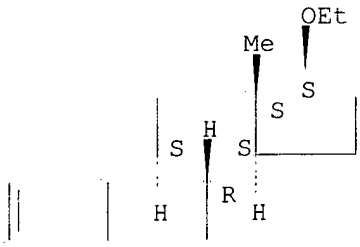
```
L64             3 S L63

     FILE 'HCAPLUS' ENTERED AT 11:45:28 ON 29 MAY 2002
L65            17 S L63

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:45:34 ON 29 MAY 2002
L66             4 S L63

     FILE 'REGISTRY' ENTERED AT 11:45:42 ON 29 MAY 2002

=> fil uspatall
FILE 'USPATFULL' ENTERED AT 11:45:59 ON 29 MAY 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 11:45:59 ON 29 MAY 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

=> d l66 bib abs hitstr tot

L66 ANSWER 1 OF 4  USPATFULL
AN     2002:61264  USPATFULL
TI     Alkyl ether modified polycyclic compounds having a terminal phenol and
       uses for protection of cells
IN     Prokai, Laszlo, Gainesville, FL, UNITED STATES
       Simpkins, James W., Fort Worth, TX, UNITED STATES
PI     US 2002035100      A1   20020321
AI     US 2001-893324     A1   20010627 (9)
PRAI   US 2000-214077P     20000627 (60)
DT     Utility
FS     APPLICATION
LREP   BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618
CLMN   Number of Claims: 46
ECL    Exemplary Claim: 1
DRWN   5 Drawing Page(s)
LN.CNT 951
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB     Methods and compositions are provided for achieving a cytoprotective
       effect by selecting a polycyclic compound with a phenol group at one end
       of the molecule and a carbon ring at the other such that an alkyl ether
       functional group in which the alkyl group has a formula
       C.sub.nH.sub.2n+1 (where n is at least 3 and less than 20) is positioned
       on the carbon ring. The compound may be used to achieve a cytoprotective
       effect in cells and to retard the development of a degenerative
       condition in a subject suffering from a disease, trauma or aging.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT  4954-12-5P 319427-03-7P
      (prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for
      cytoprotective activity of cells from degeneration)
RN   4954-12-5  USPATFULL
CN   Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI)  (CA INDEX
     NAME)

     Absolute stereochemistry.
```



HO

RN 319427-03-7 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

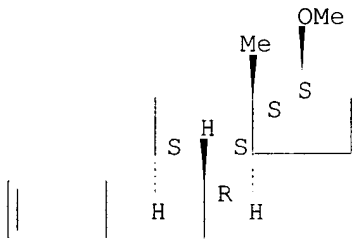
Absolute stereochemistry.



HO

IT **141318-37-8P 319426-98-7P 319426-99-8P**
319427-00-4P 319427-01-5P 319427-02-6P
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
RN 141318-37-8 USPATFULL
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

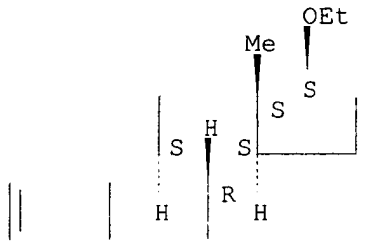
Absolute stereochemistry.



Ph O

RN 319426-98-7 USPATFULL
CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

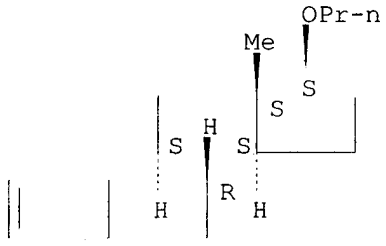
Absolute stereochemistry.



Ph O

RN 319426-99-8 USPATFULL
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

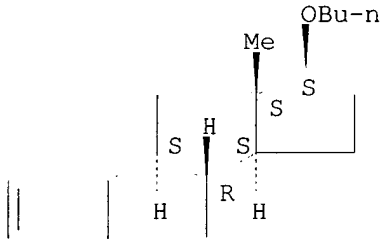
Absolute stereochemistry.



Ph O

RN 319427-00-4 USPATFULL
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

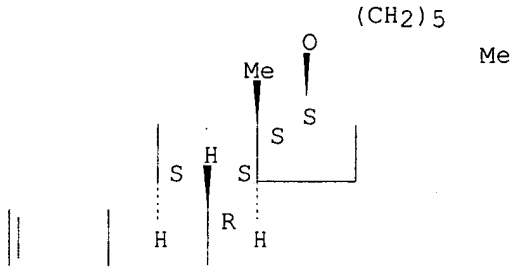
Absolute stereochemistry.



Ph O

RN 319427-01-5 USPATFULL
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

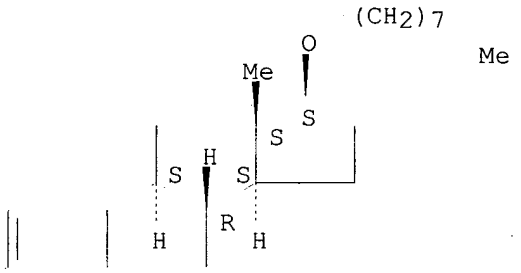
Absolute stereochemistry.



Ph O

RN 319427-02-6 USPATFULL
CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

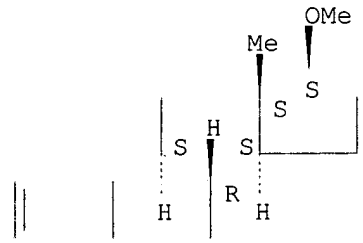


Ph O

L66 ANSWER 2 OF 4 USPATFULL
AN 1999:7375 USPATFULL
TI Steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Mountain View, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 5861388 19990119
AI US 1997-1601 19971231
RLI Division of Ser. No. US 1997-794229, filed on 29 Jan 1997, now patented, Pat. No. US 5763432
DT Utility
FS Granted
EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Bodio, Barbara
LREP Reed, Dianne E.Bozicevic & Reed LLP
CLMN Number of Claims: 22
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 1778
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) ##STR1## wherein X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **4954-12-5**
(prepn. of steroid inhibitors of estrone sulfatase)
RN 4954-12-5 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

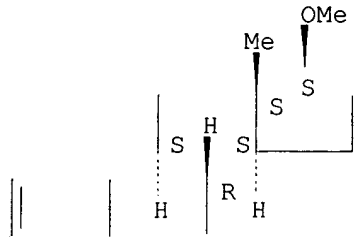
Absolute stereochemistry.



L66 ANSWER 3 OF 4 USPATFULL
AN 1998:65215 USPATFULL
TI Steriod inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Mountain View, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 5763432 19980609
AI US 1997-794229 19970129 (8)
DT Utility
FS Granted
EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Badio, Barbara
LREP Reed, Dianne E.Bozicevic & Reed LLP
CLMN Number of Claims: 13
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 1700
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) ##STR1## wherein X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **4954-12-5**
(prepn. of steroid inhibitors of estrone sulfatase)
RN 4954-12-5 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

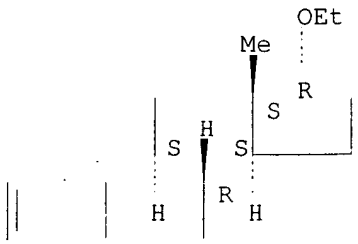


HO

L66 ANSWER 4 OF 4 USPATFULL
AN 96:82674 USPATFULL
TI Methods for neuroprotection
IN Simpkins, James W., Gainesville, FL, United States
Singh, Meharvan, Gainesville, FL, United States
Bishop, Jean, Jacksonville, FL, United States
PA University of Florida, Gainesville, FL, United States (U.S. corporation)
PI US 5554601 19960910
AI US 1994-318042 19941004 (8)
RLI Continuation-in-part of Ser. No. US 1993-149175, filed on 5 Nov 1993, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Weddington, Kevin E.
LREP Bromberg & Sunstein
CLMN Number of Claims: 29
ECL Exemplary Claim: 1
DRWN 11 Drawing Figure(s); 10 Drawing Page(s)
LN.CNT 1532
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A method is provided for conferring neuroprotection on a population of cells using estrogen compounds that have insubstantial sex activity and furthermore, a method is provided that utilizes estrogen compounds in the absence of testosterone for treating neurodegenerative diseases including Alzheimer's disease so as to retard the adverse effects of these disorders, Examples of estrogen compounds that have insubstantial sex activity includes alpha isomers of estrogen compounds such as 17.alpha. estradiol.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **182624-49-3 182624-51-7 182823-27-4**
(methods for neuroprotection)
RN 182624-49-3 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.alpha.)- (9CI) (CA INDEX NAME)

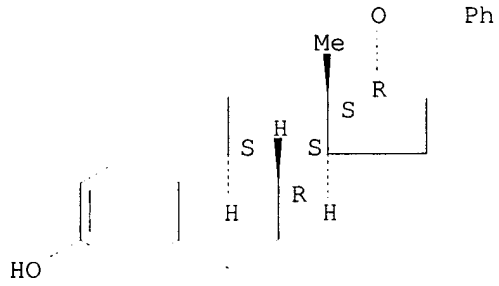
Absolute stereochemistry.



HO

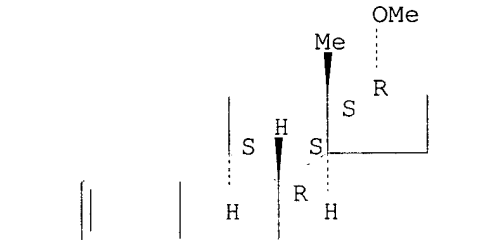
RN 182624-51-7 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 182823-27-4 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 11:46:09 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 29 May 2002 VOL 136 ISS 22
FILE LAST UPDATED: 27 May 2002 (20020527/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

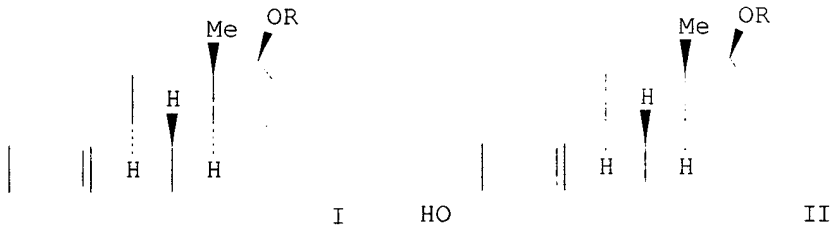
CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d l65 all hitstr tot

L65 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:10439 HCAPLUS
DN 136:85991
TI Preparation of 17.beta.-alkyl ether estradiol derivatives with cytoprotective activity of cells from degeneration through disease, trauma or aging
IN Prokai, Laszlo; Simpkins, James W.
PA University of Florida Research Foundation, Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002000619	A2	20020103	WO 2001-US41170	20010627
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002035100	A1	20020321	US 2001-893324	20010627
PRAI US 2000-214077P	P	20000627		

GI



AB Cytoprotective compds. I (R = Me, Et, Pr, Bu, (CH2)5Me, or (CH2)7Me; R1 = OH) were prepd. in 50-75% yields from 17.beta.-estradiol. 17.beta.-Estradiol and benzyl halide in K2CO3 gave 93% yield of 3-benzyloxyestra-1,3,5(10)-trien-17.beta.-ol which was then alkylated with the appropriate alkyl halides in DMF and NaH yielding the 3-benzyloxy protected derivs. of I which were then deprotected via catalytic hydrogenation using ammonium formate in Pd/C. Thus compds. II (R = hexyl and octyl) were prepd. in 70 and 75% resp., and were neuroprotective to a similar extent at a concn. of 10 .mu.M and 1 .mu.M. Typical compns. contain approx. 0.01-95% by wt. of active ingredient and the percentage of active ingredient will depend upon the dosage form and mode of administration; an ED of the active agent as measured in the plasma of a

subject may be in the range of 5pg/mL-5000pg/mL. Cytoprotective compds. I (R = OH; R1 = Bu, (CH2)7Me) were prepd. from 17.beta.-estradiol and Bu or octyl bromide in K2CO3 in 68 and 72% resp.

ST estradiol hydroxy alkylated deriv prepn cytoprotective compn; neuroprotective alkyl ether steroid prepn; crystal structure butoxyestratrienol

IT Steroids, preparation
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(alkylation of 17.beta.-OH or 3-OH; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Cytoprotective agents
(cardioprotective; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Nervous system
(degeneration; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Alkylation
(hydroxyalkylation; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Eye, disease
(macula, degeneration; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Crystal structure
(of 17.beta.-butoxyestra-1,3,5(10)-trien-3-ol)

IT Estrogen receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used as cytoprotective agents of cells from degeneration)

IT Anti-Alzheimer's agents
Anti-ischemic agents
Bone, disease
Drug delivery systems
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Osteoporosis
(therapeutic agents; prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT 319427-05-9P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure)

IT **4954-12-5P** 21830-24-0P 128805-68-5P **319427-03-7P**
319427-04-8P 319427-06-0P 319427-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT 50-28-2, 17.beta.-Estradiol, reactions 109-65-9, Butyl bromide 111-83-1, Octyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT 14982-15-1P **141318-37-8P 319426-98-7P**
319426-99-8P 319427-00-4P 319427-01-5P
319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for

cytoprotective activity of cells from degeneration)

IT **4954-12-5P 319427-03-7P**

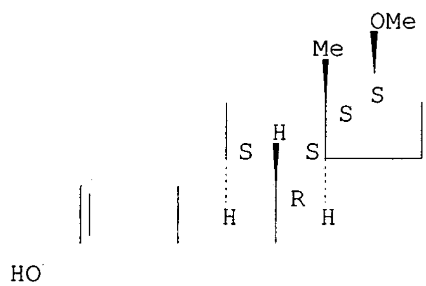
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

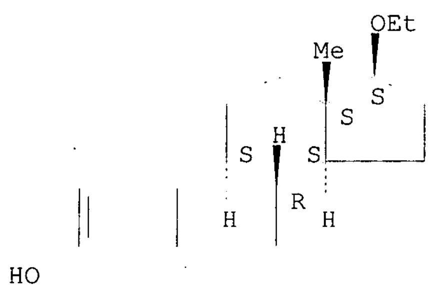
Absolute stereochemistry.



RN 319427-03-7 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **141318-37-8P 319426-98-7P 319426-99-8P 319427-00-4P 319427-01-5P 319427-02-6P**

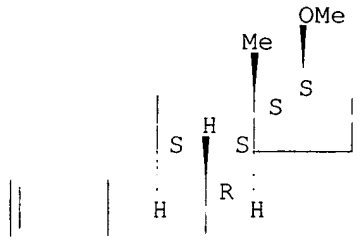
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

RN 141318-37-8 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

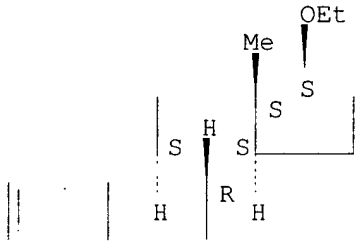
Absolute stereochemistry.



Ph O

RN 319426-98-7 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

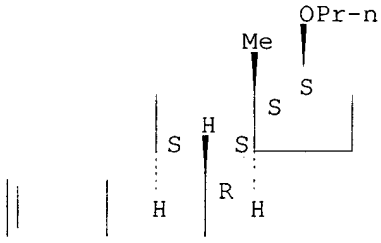
Absolute stereochemistry.



Ph O

RN 319426-99-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

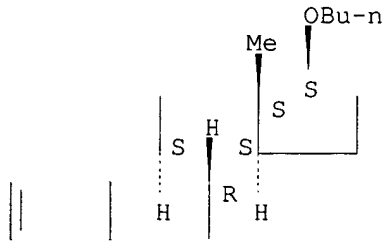
Absolute stereochemistry.



Ph O

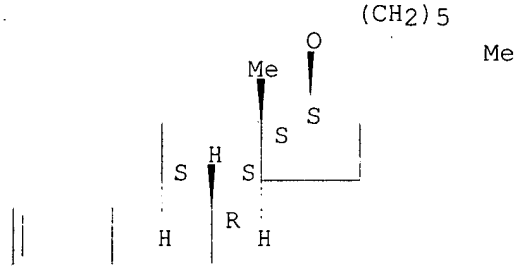
RN 319427-00-4 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



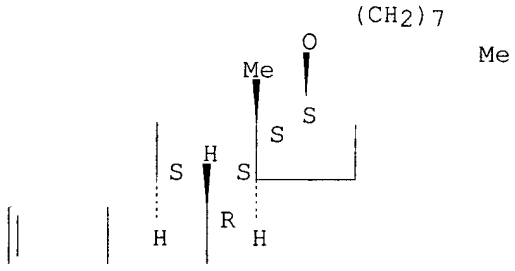
RN 319427-01-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-02-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 2000:820327 HCAPLUS
DN 134:101056
TI Synthesis and Biological Evaluation of 17.beta.-Alkoxyestra-1,3,5(10)-trienes as Potential Neuroprotectants Against Oxidative Stress
AU Prokai, Laszlo; Oon, Su-Min; Prokai-Tatrai, Katalin; Abboud, Khalil A.; Simpkins, James W.
CS Center for Drug Discovery College of Pharmacy Department of Anesthesiology College of Medicine and Center for Neurobiology of Aging College of Pharmacy, University of Florida, Gainesville, FL, 32610-0497, USA
SO Journal of Medicinal Chemistry (2001), 44(1), 110-114

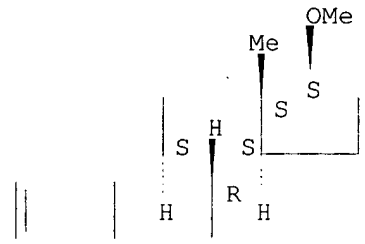
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
OS CASREACT 134:101056
AB 17.beta.-O-Alkyl ethers (Me, Et, Pr, Bu, hexyl, and octyl) of estradiol were obtained from 3-O-benzyl-17.beta.-estradiol with sodium hydride/alkyl halide, followed by the removal of the O-benzyl protecting group via catalytic transfer hydrogenation. An increase compared to estradiol in the protection of neural (HT-22) cells against oxidative stress due to exposure of glutamate was furnished by higher (C-3 to C-8) alkyl ethers, while Me and Et ethers decreased the neuroprotective effect significantly. Lipophilic (Bu and octyl) ethers blocking the phenolic hydroxyl (3-OH) of A-ring were inactive.
ST alkoxyestratriene prepn neuroprotectant oxidative stress; estratriene alkoxy prepn neuroprotectant oxidative stress
IT Cytoprotective agents
(neuroprotectants; synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT Crystal structure
Molecular structure
Oxidative stress, biological
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT 319427-05-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT **4954-12-5P** 21830-24-0P 128805-68-5P **319427-03-7P**
319427-04-8P 319427-06-0P 319427-07-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT 50-28-2, 17.beta.-Estradiol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT 14982-15-1P **141318-37-8P 319426-98-7P**
319426-99-8P 319427-00-4P 319427-01-5P
319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anwer, M; Synthesis 1980, P929 HCAPLUS
(2) Behl, C; Biochem Biophys Res Commun 1995, V216, P473 HCAPLUS
(3) Behl, C; Cell 1994, V77, P817 HCAPLUS
(4) Behl, C; Mol Pharmacol 1997, V51, P535 HCAPLUS

(5) Bishop, J; Mol Cell Neurosci 1994, V5, P303 HCAPLUS
(6) Coombs, M; Steroids 1965, V6, P841 HCAPLUS
(7) Elamin, B; J Org Chem 1979, V44, P3442 HCAPLUS
(8) Ghose, A; J Comput Chem 1988, V9, P80 HCAPLUS
(9) Glenner, G; Cell 1988, V52, P307 HCAPLUS
(10) Green, P; J Neurocytol, in press
(11) Green, P; J Neurosci 1997, V17, P511 HCAPLUS
(12) Green, P; J Steroid Biochem Mol Biol 1997, V63, P229 HCAPLUS
(13) Green, P; Neurosci Lett 1996, V218, P165 HCAPLUS
(14) Green, P; Neuroscience 1998, V84, P7 HCAPLUS
(15) Gridley, K; Mol Pharmacol 1998, V54, P874 HCAPLUS
(16) Kawas, C; Neurology 1997, V48, P1517 HCAPLUS
(17) Maher, P; J Neurosci 1996, V15, P6394
(18) Mook-Jung, I; Neurosci Lett 1997, V235, P101 HCAPLUS
(19) Moorsmann, B; Proc Natl Acad Sci U S A 1999, V96, P8867
(20) Paganni-Hill, A; Am J Epidemiol 1994, V140, P256
(21) Pike, J; J Neurochem 1999, V72, P1552
(22) Qian, X; J Steroid Biochem 1988, V29, P657 HCAPLUS
(23) Sawada, H; J Neurosci Res 1998, V54, P707 HCAPLUS
(24) Shearman, M; Proc Natl Acad Sci U S A 1994, V91, P470
(25) Sheldrick, G; SHELXTL5 1998
(26) Yankner, B; Neuron 1996, V16, P921 HCAPLUS

IT **4954-12-5P 319427-03-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

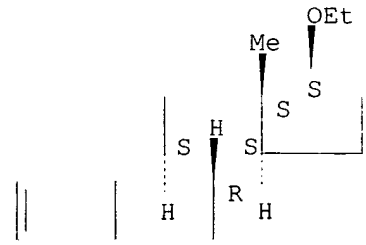
Absolute stereochemistry.



HO

RN 319427-03-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

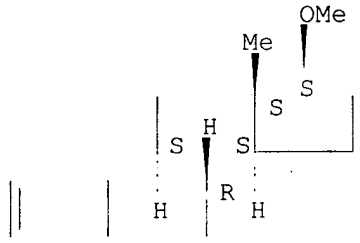


HO

IT **141318-37-8P 319426-98-7P 319426-99-8P**
319427-00-4P 319427-01-5P 319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17.beta.-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RN 141318-37-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

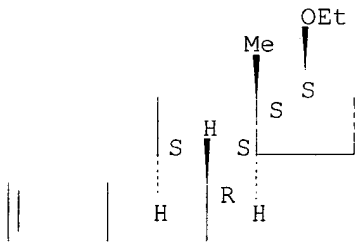
Absolute stereochemistry.



Ph O

RN 319426-98-7 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

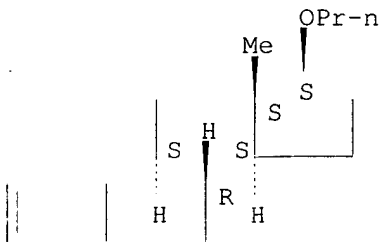
Absolute stereochemistry.



Ph O

RN 319426-99-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

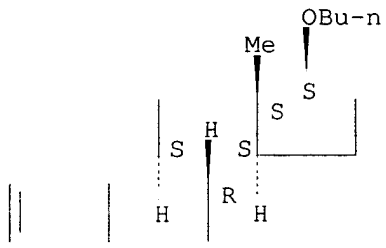
Absolute stereochemistry.



Ph O

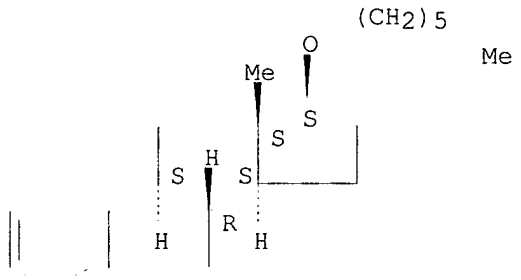
RN 319427-00-4 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



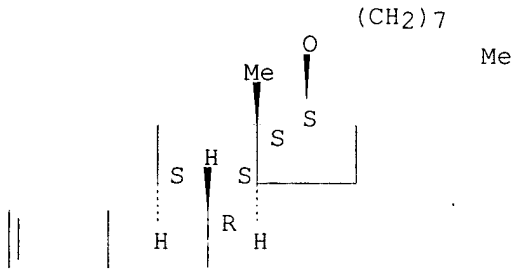
RN 319427-01-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-02-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1999:30570 HCAPLUS
DN 130:293190
TI Human 17.beta.-hydroxysteroid dehydrogenase-ligand complexes: crystals of different space groups with various cations and combined seeding and co-crystallization
AU Zhu, D.-W.; Han, Q.; Qiu, W.; Campbell, R. L.; Xie, B.-X.; Azzi, A.; Lin, S.-X.
CS CHUL Research Center, Medical Research Council Group in Molecular

Endocrinology, Laval University, Quebec, G1V 4G2, Can.
SO Journal of Crystal Growth (1999), 196(2-4), 356-364
CODEN: JCRGAE; ISSN: 0022-0248
PB Elsevier Science B.V.
DT Journal
LA English
CC 7-5 (Enzymes)
Section cross-reference(s): 75
AB Human estrogenic 17.beta.-hydroxysteroid dehydrogenase (17.beta.-HSD1) is responsible for the synthesis of active estrogens that stimulate the proliferation of breast cancer cells. The enzyme has been crystd. using a Mg2+/PEG (3500)/.beta.-octyl glucoside system. The space group of these crystals is C2. Here we report that cations can affect 17.beta.-HSD1 crystn. significantly. In the presence of Mn2+ instead of Mg2+, crystals have been obtained in the same space group with similar unit cell dimensions. In the presence of Li+ and Na+ instead of Mg2+, the space group has been changed to P212121. A whole data set for a crystal of 17.beta.-HSD1 complex with progesterone grown in the presence of Li+ has been collected to 1.95 .ANG. resoln. with a synchrotron source. The cell dimensions are a=41.91 .ANG., b=108.21 .ANG., c=117.00 .ANG.. The structure has been preliminarily detd. by mol. replacement, yielding important information on crystal packing in the presence of different cations. In order to further understand the structure-function relationship of 17.beta.-HSD1, enzyme complexes with several ligands have been crystd. As the steroids have very low aq. soly., we used a combined method of seeding and co-crystn. to obtain crystals of 17.beta.-HSD1 complexed with various ligands. This method provides ideal conditions for growing complex crystals, with ligands such as 20.alpha.-hydroxysteroid progesterone, testosterone and 17.beta.-methyl-estradiol-NADP+. Several complex structures have been detd. with reliable electronic d. of the bound ligands.
ST hydroxysteroid dehydrogenase ligand complex crystn human; crystal structure hydroxysteroid dehydrogenase ligand complex human
IT Cations
Crystal growth
Crystal structure
(crystals of human 17.beta.-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)
IT 9028-61-9, 17.beta.-Estradiol dehydrogenase
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(crystals of human 17.beta.-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)
IT 53-59-8DP, Nadp, complexes with 17.beta.-hydroxysteroid dehydrogenase and 17.beta.-methylestradiol 58-22-0DP, Testosterone, complexes with 17.beta.-hydroxysteroid dehydrogenase 145-14-2DP, 20.alpha.-HydroxyProgesterone, complexes with 17.beta.-hydroxysteroid dehydrogenase **4954-12-5DP**, complexes with 17.beta.-hydroxysteroid dehydrogenase and NADP 9028-61-9DP, 17.beta.-Estradiol dehydrogenase, ligand complexes
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(crystals of human 17.beta.-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Azzi, A; Nature Struct Biol 1996, V3, P665 HCAPLUS
(2) Breton, R; J Steroid Biochem Mol Biol 1994, V50, P275 HCAPLUS
(3) Breton, R; Structure 1996, V8, P905
(4) Chin, C; Steroid 1973, V22, P373 HCAPLUS
(5) Crosio, M; J Mol Biol 1992, V228, P243 HCAPLUS
(6) Descomps, B; Bull Soc Chim Biol 1968, V50, P1681 HCAPLUS
(7) Geissler, W; Nat Genet 1994, V7, P34 HCAPLUS
(8) Ghosh, D; Structure 1995, V5, P503
(9) Han, Q; J Crystal Growth 1996, V168, P181 HCAPLUS

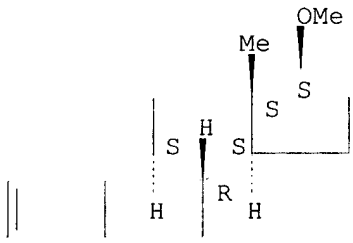
(10) Jarabak, J; Methods Enzymol 1969, V15, P746 HCAPLUS
(11) Labrie, F; Endocrine Rev 1986, V7, P67 MEDLINE
(12) Labrie, F; Steroids 1997, V62, P148 HCAPLUS
(13) Lim, K; The Abstract of 7th Int Conf on the Crystallization of Biological Macromolecules 1998, P98
(14) Lin, S; J Biol Chem 1992, V267, P16182 HCAPLUS
(15) Lin, S; J Endocrinol 1996, V150, P513
(16) Luu-The, V; Mol Endocrinol 1989, V3, P1301
(17) Martel, C; J Steroid Biochem Mol Biol 1992, V41, P597 HCAPLUS
(18) Murdock, G; Biochemistry 1986, V25, P641 HCAPLUS
(19) Otwinowski, M; Methods in Enzymology 1996, P276
(20) Peltoketo, H; FEBS Lett 1988, V239, P73 HCAPLUS
(21) Poulin, R; Cancer Res 1986, V46, P4933 HCAPLUS
(22) Stura, E; Crystallization of Nucleic Acids and proteins 1992, P99 HCAPLUS
(23) Wu, L; J Biol Chem 1993, V268, P12964 HCAPLUS
(24) Zhu, D; Acta Crystallogr D 1994, V50, P550
(25) Zhu, D; J Crystal Growth 1996, V168, P272
(26) Zhu, D; J Mol Biol 1993, V234, P242 HCAPLUS

IT **4954-12-5DP**, complexes with 17.beta.-hydroxysteroid dehydrogenase and NADP
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(crystals of human 17.beta.-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2002 ACS

AN 1998:397783 HCAPLUS

DN 129:54482

TI Preparation of steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use

IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Shigeno, Kazuhiko

PA SRI International, USA

SO U.S., 23 pp.
CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-58
ICS C07J071-00

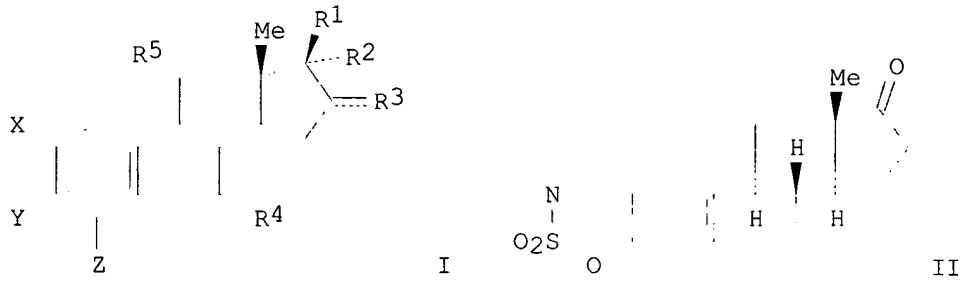
NCL 514176000

CC 32-3 (Steroids)
Section cross-reference(s): 1, 2

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5763432	A	19980609	US 1997-794229	19970129
	US 5861388	A	19990119	US 1997-1601	19971231

WO 9832763 A1 19980730 WO 1998-US1846 19980129
W: CA, JP, KR
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
PRAI US 1997-794229 19970129
OS MARPAT 129:54482
GI



AB Estratriene derivs. of formula I [X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring; R1, R2 = H, alkyl, alkynyl, (substituted) OH; R1R2 = O, S, (substituted) CH2; R3 = H, halo, alkyl, CH2; R4 = H, alkyl; R5 = H, OH, alkyl, alkenyl, alkoxy, aryl, CH2] are prepd. as inhibitors of estrone sulfatase. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided as well. Thus, estradiol is transformed into II in 3 steps. In an estrone sulfatase inhibition assay, II showed 5-% inhibition at 9.3 nM.

ST estratriene deriv prepn estrone sulfatase inhibitor

IT 208758-20-7P 208758-22-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of steroid inhibitors of estrone sulfatase)

IT 208758-16-1P 208758-17-2P 208758-21-8P 208758-23-0P 208758-25-2P
208758-33-2P 208758-34-3P 208758-35-4P 208758-36-5P 208758-37-6P
208758-38-7P 208758-39-8P 208758-41-2P 208758-43-4P 208758-48-9P
208758-52-5P 208758-54-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of steroid inhibitors of estrone sulfatase)

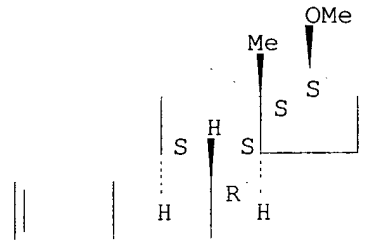
IT 59298-96-3, Estrone sulfatase
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(prepn. of steroid inhibitors of estrone sulfatase)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, 17.alpha.-Ethynylestradiol 1530-32-1, Ethyltriphenylphosphonium bromide 1779-51-7, Butyltriphenylphosphonium bromide **4954-12-5** 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 59077-04-2, 19-Norpregna-1,3,5(10)-trien-3-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of steroid inhibitors of estrone sulfatase)

IT 4736-62-3P 6599-97-9P 13879-55-5P 13879-56-6P 31559-62-3P
34111-53-0P 57711-40-7P 64215-82-3P 99898-93-8P 120574-27-8P
120574-28-9P 123715-79-7P 137352-12-6P 206442-55-9P 208758-18-3P
208758-19-4P 208758-24-1P 208758-26-3P 208758-27-4P 208758-28-5P
208758-29-6P 208758-30-9P 208758-31-0P 208758-32-1P 208758-40-1P
208758-42-3P 208758-44-5P 208758-45-6P 208758-46-7P 208758-47-8P
208758-50-3P 208758-51-4P 208758-53-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(prepn. of steroid inhibitors of estrone sulfatase)
IT 208758-49-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of steroid inhibitors of estrone sulfatase)
IT **4954-12-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of steroid inhibitors of estrone sulfatase)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1996:580562 HCAPLUS
DN 125:294029
TI Methods for neuroprotection
IN Simpkins, James W.; Singh, Meharvan; Bishop, Jean
PA University of Florida, USA
SO U.S., 25 pp., Cont.-in-part of U.S. Ser. No. 149,175, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-56
NCL 514182000
CC 2-4 (Mammalian Hormones)
FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5554601	A	19960910	US 1994-318042	19941004
	CA 2175603	AA	19950511	CA 1994-2175603	19941107
	WO 9512402	A1	19950511	WO 1994-US12782	19941107
	W: AU, CA, JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9510901	A1	19950523	AU 1995-10901	19941107
	AU 699361	B2	19981203		
	EP 799041	A1	19971008	EP 1995-901795	19941107
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
	JP 11514327	T2	19991207	JP 1994-513454	19941107
	US 5843934	A	19981201	US 1996-648857	19960516
	US 5877169	A	19990302	US 1996-749703	19961115
	US 6319914	B1	20011120	US 1999-351492	19990712
PRAI	US 1993-149175	B2	19931105		
	US 1994-318042	A	19941004		
	WO 1994-US12782	W	19941107		
	US 1996-648857	A2	19960516		
	US 1996-685574	A2	19960724		
	US 1996-749703	A3	19961115		
	US 1997-782883	A3	19970110		

US 1998-128862 A3 19980804
US 1998-129209 A2 19980804
US 1998-179640 A3 19981027

AB A method is provided for conferring neuroprotection on a population of cells using estrogen compds. that have insubstantial sex activity and furthermore, a method is provided that utilizes estrogen compds. in the absence of testosterone for treating neurodegenerative diseases including Alzheimer's disease to retard the adverse effects of these disorders, Examples of estrogen compds. that have insubstantial sex activity includes alpha isomers of estrogen compds. such as 17.alpha.-estradiol.

ST estrogen neuroprotection

IT Nerve
(methods for neuroprotection)

IT Estrogens
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for neuroprotection)

IT Molecular structure-biological activity relationship
(neuroprotective; methods for neuroprotection)

IT Mental disorder
(Alzheimer's disease, methods for neuroprotection)

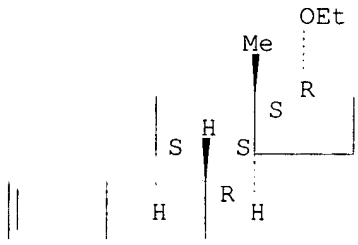
IT 53-16-7, biological studies 57-63-6, 17.alpha.-Ethynylestradiol 57-91-0, 17.alpha.-Estradiol 10093-54-6 15068-99-2 33602-53-8 65684-87-9 110114-70-0 **182624-49-3** 182624-50-6 **182624-51-7** 182624-52-8 182624-53-9 182624-54-0 182624-55-1 182624-56-2 182624-57-3 182624-58-4 182624-59-5 182624-60-8 182624-61-9 **182823-27-4**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for neuroprotection)

IT **182624-49-3 182624-51-7 182823-27-4**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for neuroprotection)

RN 182624-49-3 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.alpha.)- (9CI) (CA INDEX NAME)

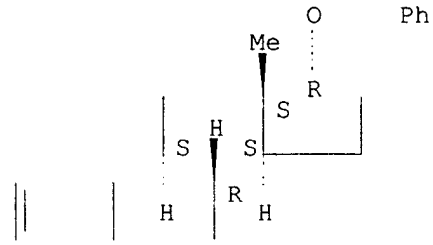
Absolute stereochemistry.



RN 182624-51-7 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17.alpha.)- (9CI) (CA INDEX NAME)

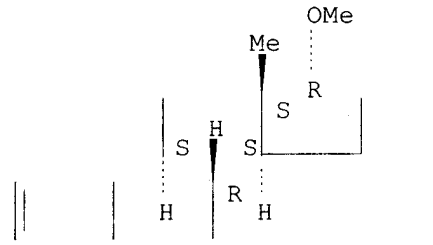
Absolute stereochemistry.



HO

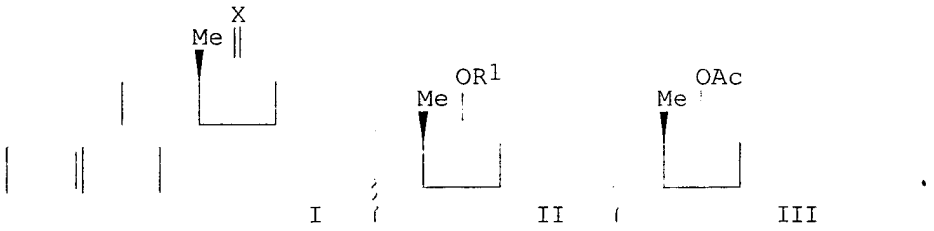
RN 182823-27-4 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

L65 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1992:235946 HCAPLUS
DN 116:235946
TI Synthesis and properties of 3,17-disubstituted estrogenic steroids
AU Tong, Z. S.; Gan, G. Z.; Li, L.; Tang, Z. M.
CS Inst. Radiat. Med., Acad. Mil. Med. Sci., Beijing, 100850, Peop. Rep. China
SO Yaoxue Xuebao (1992), 27(3), 236-40
CODEN: YHHPAL; ISSN: 0513-4870
DT Journal
LA Chinese
CC 32-3 (Steroids)
Section cross-reference(s): 8
GI



AB Ten title radioprotective estrogens, e.g., I [R = H, Me, cyclopentyl; X = NOMe, N(CH2)nCH2OH, n = 1, 2], II (R1 = H, Me, CH2CH2OH) and III were prepd. I [R = cyclopentyl, X = N(CH2)nCH2OH, N = 1, 2] showed better

protective effect in mice than estradiol upon 750 rad .gamma.-irradn. with 60Co. Several compds. increased 30-day survival rate by 35-80% in mice exposed to 900 rad of irradn. when administered i.p. 0.1 mg per mouse 24 h before irradn.

ST estratrienol prepn radioprotectant

IT Radioprotectants
(estratrienols, against .gamma.-rays)

IT **141318-37-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation of)

IT 14982-15-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and methylation of)

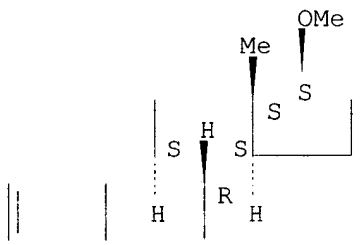
IT 2774-51-8P **4954-12-5P** 6038-28-4P 27543-03-9P 94514-10-0P 94514-11-1P 94514-13-3P 94514-15-5P 94876-43-4P 97117-16-3P 141276-94-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and radioprotective activity of)

IT **141318-37-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation of)

RN 141318-37-8 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



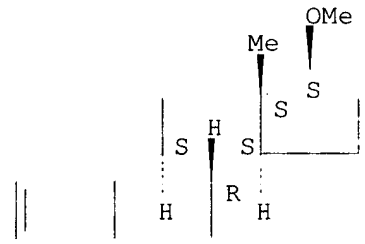
Ph O

IT **4954-12-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and radioprotective activity of)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

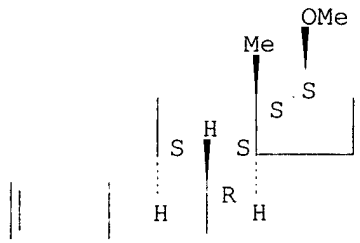
L65 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2002 ACS

AN 1984:96847 HCAPLUS

DN 100:96847
TI Specificity of an estrogen binding protein in the human vagina compared with that of estrogen receptors in different tissues from different species
AU Bergink, E. W.; Kloosterboer, H. J.; Van der Velden, W. H. M.; Van der Vies, J.; De Winter, M. S.
CS Sci. Dev. Group, Organon Int. B.V., Oss, Neth.
SO Prog. Cancer Res. Ther. (1983), 25(Steroids Endometrial Cancer), 77-84
CODEN: PCRTDK; ISSN: 0145-3726
DT Journal
LA English
CC 2-2 (Mammalian Hormones)
AB Estrogen-binding proteins from the myometrium, pituitary, thymus, and vagina of the rabbit; myometrium, endometrium, and vagina of the rat; and myometrium, breast tumor tissue, and MCF-7 cells of the human all displayed similar specificities with characteristics of an estrogen receptor. However, the specificity of the estrogen-binding protein in the human vagina was different from that of the human estrogen receptor; the estrogen-binding protein displayed high affinities for 17.beta.-estradiol [50-28-2], 17.alpha.-estradiol [57-91-0], and estriol [50-27-1], but a relatively low affinity for stilbestrol [56-53-1]. Structural requirements of estrogens for binding to the estrogen receptor in the rabbit myometrium were detd. and discussed.
ST estrogen binding protein vagina; receptor estrogen structure activity
IT Receptors
RL: BIOL (Biological study)
(estrogen binding by, in human and lab. animal, structure in relation to)
IT Neoplasm, composition
(estrogen receptor of, of mammary gland of human, specificity of)
IT Pituitary gland
Thymus gland
(estrogen receptor of, specificity of)
IT Vagina
(estrogen-binding protein of, of human and lab. animal, specificity of)
IT Estrogens
RL: PROC (Process)
(receptor binding of, in human and lab. animal, structure in relation to)
IT Molecular structure-biological activity relationship
(estrogen receptor-binding, of estrogens, in human and lab. animal)
IT Proteins
RL: BIOL (Biological study)
(estrogen-binding, of vagina, of human, specificity of)
IT Uterus, composition
(myometrium, estrogen receptor of, of human and lab. animal)
IT Mammary gland
(neoplasm, estrogen receptor of, of human, specificity of)
IT 50-27-1 50-28-2, biological studies 52-76-6 52-77-7 53-63-4
56-53-1 57-63-6 57-91-0 72-33-3 302-76-1 362-05-0 570-30-9
1035-77-4 1162-60-3 1229-24-9 1231-93-2 1464-61-5 1818-12-8
2529-54-6 2529-64-8 3398-11-6 3597-38-4 3704-15-2
4954-12-5 5444-22-4 6544-69-0 10448-97-2 10540-29-1
13570-81-5 13655-95-3 23637-93-6 34816-55-2 54502-78-2
54567-02-1 58212-59-2 58212-69-4 59077-04-2 66463-44-3
88899-71-2 88899-72-3 88899-73-4 88899-74-5 88899-75-6
88899-76-7 88930-00-1 88930-01-2
RL: PROC (Process)
(estrogen receptor binding of, in human and lab. animals, structure in relation to)
IT **4954-12-5**
RL: PROC (Process)
(estrogen receptor binding of, in human and lab. animals, structure in

relation to)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

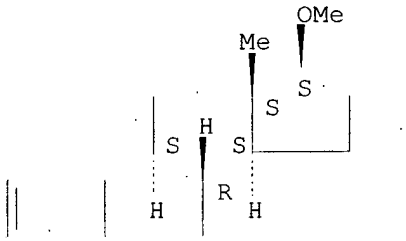
Absolute stereochemistry.



L65 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1978:402201 HCAPLUS
DN 89:2201
TI Structural requirements for maximal inhibitory allosteric effect of estrogens and estrogen analogs on glutamate dehydrogenase
AU Pons, Michel; Michel, Francoise; Descomps, Bernard; Crastes de Paulet, Andre
CS Unite Rech. Biochim. Steroides, INSERM, Montpellier, Fr.
SO Eur. J. Biochem. (1978), 84(1), 257-66
CODEN: EJBCAI; ISSN: 0014-2956
DT Journal
LA English
CC 7-3 (Enzymes)
AB The inhibition of glutamate dehydrogenase by estrogens, estrogen analogs, or polyphenylethylene derivs. (.apprx.100 mols., most of them having estrogenic or antiestrogenic activities) was measured. The efficiency of these compds. in inducing allosteric inhibition of the enzyme was compared and correlated to their chem. structure: an arom. ring A, a free phenolic group in the region of C-3 of the steroid nucleus, and a lipophilic substitution in the region of C-12, C-13, or C-17 were the main structural features required for max. efficiency on glutamate dehydrogenase. A tentative model for the relative orientation of the main inhibitor families is proposed. It accounts for most of the kinetic results and can be used as a tool for the selection of affinity labels directed towards the estrogen binding site of glutamate dehydrogenase.
ST glutamate dehydrogenase inhibition estrogen
IT Estrogens
RL: BIOL (Biological study)
(glutamate dehydrogenase inhibition by)
IT Kinetics, enzymic
(of inhibition, of glutamate dehydrogenase)
IT Molecular structure-biological activity relationship
(glutamate dehydrogenase-inhibiting, of estrogens and analogs)
IT 50-27-1 50-28-2, biological studies 53-16-7, biological studies
53-63-4 56-53-1 57-63-6 57-91-0 302-76-1 481-97-0 517-04-4
517-09-9 547-81-9 566-76-7 571-92-6 1035-77-4 1089-78-7
1213-46-3 1667-98-7 1743-60-8 1818-12-8 3398-11-6 3398-12-7
3434-88-6 3597-38-4 3736-22-9 4019-92-5 4245-41-4
4954-12-5 5189-40-2 5444-22-4 5864-38-0 5965-06-0
5976-63-6 5976-73-8 6544-69-0 10161-33-8 10218-59-4 10448-97-2
13010-22-5 13565-53-2 13864-49-8 14418-02-1 14984-42-0
14984-43-1 20796-59-2 21507-14-2 21507-16-4 21583-10-8
22831-81-8 25547-76-6 32295-36-6 33526-45-3 34816-55-2

40128-89-0 41164-28-7 53177-70-1 60973-93-5 61665-15-4
62013-77-8 65928-98-5 65929-00-2 66320-32-9 66422-07-9
66422-09-1 66422-11-5 66422-12-6 66422-14-8 66422-17-1
66422-18-2 66463-40-9 66463-41-0 66463-42-1 66463-43-2
66463-44-3 66463-45-4 66463-46-5 66463-47-6 66463-48-7
66463-49-8 66463-50-1 66495-43-0 66514-24-7 66514-25-8
66514-26-9 66514-27-0 66537-38-0
RL: BIOL (Biological study)
(glutamate dehydrogenase inhibition by)
IT 9029-12-3
RL: PROC (Process)
(inhibition of, by estrogens and analogs)
IT **4954-12-5**
RL: BIOL (Biological study)
(glutamate dehydrogenase inhibition by)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

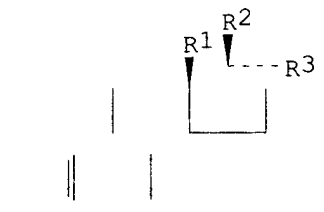
Absolute stereochemistry.



L65 ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1977:90134 HCAPLUS
DN 86:90134
TI Esterification of phenolic hydroxyl groups in steroids
IN Schwarz, Sigfrid; Weber, Gisela
PA E. Ger.
SO Ger. (East), 5 pp. Addn. to Ger.(East) 114,806.
CODEN: GEXXA8
DT Patent
LA German
IC C07C167-28
CC 32-3 (Steroids)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DD 120016	Y	19760520	DD 1975-184239	19750217

GI



I

AB Estratrienyl sulfonates I [R = R4SO2, (R4 = Me2CH, PhCH2, Me(CH2)7, 4-MeC6H4, cyclopentyl, cyclohexyl); R1 = H, Me, R2R3 = O, MeON; R2 = HO, MeO, Me3SiO, BuCO2, EtCO2, PhCH2CH2CO2, CH2:CHCH2O; R2 = H, HC.tplbond.C, ClC.tplbond.C, CH2:CH] (20 compds.) were prepd. in 76-97% yields by treatment of I (R = H) in H2O contg. an alkali hydroxide or an alk. earth hydroxide and a quaternary ammonium salt with R4SO2Cl. Thus, I (R = R1 = H, R2 = OH, R3 = C.tplbond.CH) in H2O-NaOH contg. (PhCH2)4N+Cl- was treated with Me2CHSO2Cl to give 80% I (R = Me2CHSO2, R1 = H, R2 = OH, R3 = C.tplbond.CH).

ST alkanesulfonate estratrienyl; sulfonation norpregnenynol; ethynylestradiol sulfonation; estradiol sulfonation; estrone sulfonation

IT 19-Norsteroids
RL: RCT (Reactant)
(3.beta.-hydroxy-17-oxygenated-1,3,5(10)-unsatd., sulfonates)

IT 28913-23-7P 28913-25-9P 29017-43-4P 29017-44-5P 29017-45-6P
32162-69-9P 38022-64-9P 38022-65-0P 42738-04-5P 42738-09-0P
42738-11-4P 54983-35-6P 55561-16-5P 55561-21-2P 55561-22-3P
55561-24-5P 55561-25-6P 55561-29-0P 55561-31-4P 61872-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 1939-99-7 4837-38-1 7795-95-1 10147-37-2 26394-17-2
RL: RCT (Reactant)
(reaction of, with estradienol)

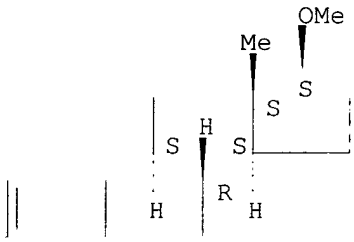
IT 50-28-2, reactions 53-16-7, reactions 57-63-6 3342-64-1 3758-34-7
4567-67-3 **4954-12-5** 7678-95-7 14012-72-7 26443-03-8
28416-77-5 33526-46-4 33760-44-0 42737-82-6 55561-41-6
RL: RCT (Reactant)
(sulfonylation of)

IT **4954-12-5**
RL: RCT (Reactant)
(sulfonylation of)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2002 ACS

AN 1975:125520 HCAPLUS

DN 82:125520

TI Steroids. 15. Sulfonyloxy derivatives of estrogens

AU Schwarz, S.; Weber, G.; Schreiber, M.

CS Wiss. Lab., VEB Jenapharm, Jena, E. Ger.

SO Pharmazie (1975), 30(1), 17-21
CODEN: PHARAT

DT Journal

LA German

CC 32-5 (Steroids)

GI For diagram(s), see printed CA Issue.

AB Estranes I (R = alkyl, cycloalkyl, CH2Ph, aminoalkyl; R1 = C.tplbond.CH, C.tplbond.CCl, CH:CH2, Et, H; R2 = OH, OSiMe3, alkoxy, acyloxy; R1R2 = O, NOH, NOSiMe3, NOAc, NOMe) (66 compds.) were prepd., e.g. by treating the 3-hydroxyestranes with RSO2Cl.

ST estrane sulfonyloxy; sulfonate estrane; norpregnatrienyl alkanesulfonate; estradiol alkanesulfonate; ethynylestradiol alkanesulfonate

IT 19-Norsteroids
RL: RCT (Reactant)
(3-hydroxy-1,3,5(10)-unsatd., sulfonated)

IT 41781-86-6
RL: RCT (Reactant)
(alkylation of)

IT 57-63-6
RL: RCT (Reactant)
(esterification of)

IT 1689-02-7 1828-66-6 10147-37-2 10539-95-4 13360-57-1 20588-68-5 26394-17-2 35856-62-3
RL: RCT (Reactant)
(esterification of 17-(trimethylsiloxy)-19-nor-17.alpha.-pregna-1,3,5(10)-trien-20-yn-3-ol by)

IT 10147-37-2
RL: RCT (Reactant)
(esterification of norpregnatrienynediol)

IT 28416-77-5
RL: RCT (Reactant)
(esterification of, with sulfonyl chlorides)

IT **4954-12-5P** 55561-41-6P 55561-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)

IT 55561-43-8P 55561-44-9P 55561-45-0P 55561-46-1P 55561-47-2P 55561-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and etherification of)

IT 55561-38-1P 55561-39-2P 55561-40-5P 55561-49-4P 55561-50-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

IT 3381-23-5P 28913-31-7P 28913-32-8P 28913-34-0P 28913-44-2P 29017-43-4P 29017-44-5P 42738-04-5P 42738-09-0P 42738-11-4P 52310-88-0P 52310-89-1P 52310-90-4P 54983-32-3P 54983-33-4P 55561-09-6P 55561-10-9P 55561-11-0P 55561-12-1P 55561-13-2P 55561-14-3P 55561-16-5P 55612-89-0P 55786-15-7P 55786-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)

IT 4236-42-4P 28913-23-7P 28913-35-1P 28913-36-2P 54983-34-5P 54983-35-6P 54983-36-7P 54983-37-8P 54983-38-9P 55561-15-4P 55561-17-6P 55561-18-7P 55561-19-8P 55561-20-1P 55561-21-2P 55561-23-4P 55561-24-5P 55561-25-6P 55561-26-7P 55561-27-8P 55561-28-9P 55561-29-0P 55561-30-3P 55561-31-4P 55561-32-5P 55561-33-6P 55561-34-7P 55561-35-8P 55561-36-9P 55561-37-0P 55561-51-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

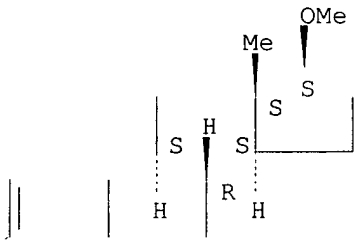
IT 55561-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., esterification, and etherification of)

IT **4954-12-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and esterification of)

RN 4954-12-5 HCAPLUS

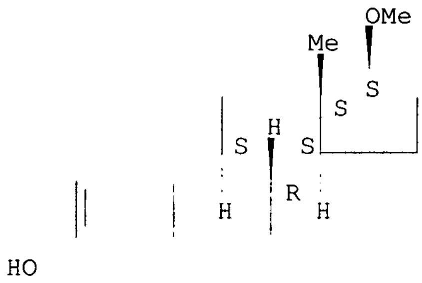
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1973:533109 HCAPLUS
DN 79:133109
TI Comparative study of estrogen action
AU Raynaud, Jean P.; Bouton, Marie M.; Gallet-Bourquin, Danielle; Philibert, Daniel; Tournemine, Colette; Azadian-Boulanger, Genevieve
CS Cent. Rech., Roussel-Uclaf, Romainville, Fr.
SO Mol. Pharmacol. (1973), 9(4), 520-33
CODEN: MOPMA3
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
AB The tissue distribution, metab., uterine uptake, and plasma and tissue binding of 8estradiol (I) [50-28-2] and 8ethynylestradiol (II) [57-63-6] derivs. were studied in rats in vivo and in vitro, and the results were related to uterotropic activity. Introduction of a methoxy group in position 11 of II, and esp. I, increased uterotropic activity, whereas methylation of OH groups in postions 3 and 17 decreased it. Uterotropic activity was directly related to binding of the compds. by the 8 S uterine cytosol receptor in vivo. Activity could not be related to binding in vitro. Binding to plasma was not a prerequisite for activity but could modulate it.
ST estradiol deriv uterotropic; ethynylestradiol deriv uterotropic; uterotropic estradiol deriv
IT Cytoplasm
(estradiol derivs. binding by, of uterus, uterotropic activity of in relation to)
IT Blood plasma
(estradiol derivs. metab. by, uterotropic activity in relation to)
IT Uterus, metabolism
(of estradiol derivs., uterotropic activity in relation to)
IT Molecular structure-biological activity relationship
(uterotropic, of estradiol derivs.)
IT 50-28-2, biological studies 57-63-6 72-33-3 1035-77-4
4954-12-5 4954-14-7 7548-45-0 21507-14-2 21507-16-4
21507-17-5 33526-45-3 33526-46-4 33526-47-5 33526-48-6
33713-12-1 34816-55-2
RL: BIOL (Biological study)
(uterotropic activity of)
IT **4954-12-5**
RL: BIOL (Biological study)
(uterotropic activity of)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

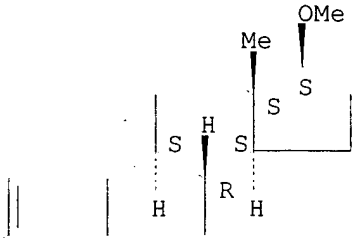
Absolute stereochemistry.



AN 1973:427594 HCAPLUS
DN 79:27594
TI Specificity of the estrogen receptor of human uterus
AU Haehnel, Roland; Twaddle, Ella; Ratajczak, Thomas
CS Dep. Obstet. Gynaecol., King Edward Mem. Hosp., Subiaco, Aust.
SO J. Steroid Biochem. (1973), 4(1), 21-31
CODEN: JSTBBK
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
AB The estrogen receptor specificity of the human uterus was detd. from the relative abilities of various steroids to compete with 17.beta.-estradiol (I) [50-28-2] for receptor sites in the uterine cytosol fraction. Highest affinity for the receptor required a free phenolic OH group on C3 and an alc. group having the .beta.-configuration at C17, the former being particularly crit. Me groups at C1 or C4 decreased the affinity drastically, whereas the effect of a Me group at C2 was relatively slight. Addnl. O functions in ring D, addnl. substituents on ring A, and unsatn. in ring B decreased the affinity for the receptor, while the presence or absence of the angular Me group at C13 had no influence.
ST steroid uterus estrogen receptor
IT Molecular structure-biological activity relationship
(estrogen receptor affinity-affecting, of steroids)
IT Uterus
(estrogen receptors of, specificity of)
IT Receptors
RL: BIOL (Biological study)
(for estrogen, of uterus, specificity of)
IT 50-23-7 50-27-1 53-16-7 53-43-0 53-45-2 53-63-4 56-53-1 57-63-6 57-83-0, biological studies 57-91-0 58-22-0 68-96-2 145-13-1 434-22-0 474-86-2 481-95-8 481-96-9 481-97-0 517-09-9 547-81-9 566-75-6 571-20-0 793-89-5 1035-77-4 1090-04-6 1150-90-9 1156-92-9 1217-09-0 1228-72-4 1229-33-0 1474-53-9 1624-62-0 1806-98-0 1818-12-8 1818-13-9 1818-29-7 1852-50-2 1852-53-5 2259-89-4 2479-91-6 2529-64-8 3232-69-7 3233-69-0 3434-88-6 3597-38-4 **4954-12-5** 5635-50-7 15093-14-8 15270-30-1 20431-33-8 20592-42-1 35577-54-9 35577-55-0 42028-17-1 42028-18-2 42028-20-6 42028-21-7
RL: BIOL (Biological study)
(estradiol binding by uterus in response to)
IT 50-28-2, biological studies
RL: BIOL (Biological study)
(receptors for, of uterus, specificity of)
IT **4954-12-5**
RL: BIOL (Biological study)
(estradiol binding by uterus in response to)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX

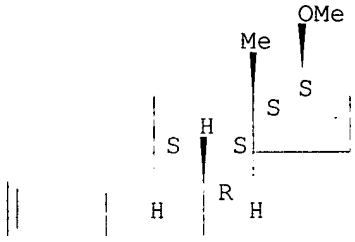
NAME)

Absolute stereochemistry.



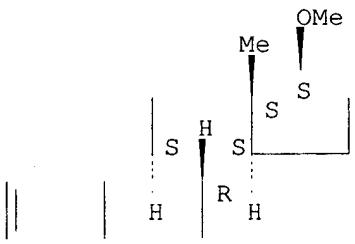
L65 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:561827 HCAPLUS
DN 77:161827
TI Degradation of steroids by intestinal bacteria. IV. Aromatization of ring A
AU Goddard, P.; Hill, M. J.
CS Bacterial. Dep., St. Mary's Hosp. Med. Sch., London, Engl.
SO Biochim. Biophys. Acta (1972), 280(2), 336-42
CODEN: BBACAQ
DT Journal
LA English
CC 10-2 (Microbial Biochemistry)
AB A strain of Escherichia coli has been shown to produce estradiol from 4-androsten-3,17-dione. From the same substrate a strain of Clostridium paraputrificum produced 17-methoxy-1,3,5(10)-estratriene-3-ol.
ST Escherichia metab androstenedione; Clostridium metab androstenedione; androstenedione bacteria intestine; steroid aromatization gut bacteria
IT Escherichia coli
(estradiol formation from androstendione by)
IT Clostridium paraputrificum
(methoxyestratrienol formation from androstenedione by)
IT 63-05-8
RL: BIOL (Biological study)
(aromatization of A of, by intestinal bacteria)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
IT 50-28-2, biological studies
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Escherichia coli)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:11880 HCAPLUS
DN 76:11880
TI Aromatization of androst-4-ene-3,17-dione by human intestinal bacteria
AU Goddard, P.; Hill, M. J.
CS Dep. Bacteriol., St. Mary's Hosp. Med. Sch., London, Engl.
SO Biochem. J. (1971), 124(5), 73P
CODEN: BIJOAK
DT Journal
LA English
CC 10 (Microbial Biochemistry)
AB Clostridium paraputrificum grown anaerobically on broth converted androst-4-ene-3,17-dione to 17.beta.-methoxyestra-1,3,5(10)-trien-3-ol by transfer of the Me group from C-10 to the oxygen on C-17 and aromatization.
ST androstenedione metab Clostridium; steroid metab Clostridium; methoxyestratrienol synthesis Clostridium; estratrienol methoxy Clostridium; androgen aromatization bacterial
IT Clostridium paraputrificum
(methoxyestratrienol formation by, from androstenedione)
IT 63-05-8
RL: RCT (Reactant)
(aromatization of, by Clostridium paraputrificum)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

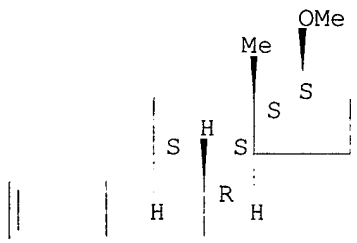
Absolute stereochemistry.



L65 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2002 ACS

AN 1971:459189 HCAPLUS
DN 75:59189
TI Pharmacodynamic model for studying the mode of action of estrogens using radioactive compounds
AU Raynaud, Jean P.; Azadian-Boulanger, Genevieve; Bourquin, Daniele; Philibert, Daniel
CS Cent. Rech. Roussel-Uclaf, Romainville, FR
SO Symp. Progr. Tech. Nucl. Pharmacodyn. (1971), Meeting Date 1970, 39-51. Editor(s): Valette, Guillaume. Publisher: Masson, Paris, Fr. CODEN: 23IDAY
DT Conference
LA French
CC 4 (Hormones and Related Substances)
AB Radioactive steroid was injected into prepubertal rats which were then sacrificed. The increased wt. of the uterus as well as its incorporation of radioactivity was measured as a function of time, 0 to 70 hr, and anal. was made of estradiol, ethynyl estradiol, and 2 other derivs. The uterus reached a max. wt. at 30-40 hr. The radioactive steroids in the uterus peaked at 1-2 hr and by 10 hr were falling, while estrogen metabolites in the plasma were rising. A math. relation between the wt. of the uterus and the concn. of steroid and metabolites is derived.
ST estrogen action mode; uterus wt estrogen; plasma metabolite estrogen
IT Estrogenic hormones
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus, mol. structure in relation to)
IT Simulation, model
(of estrogens metabolism by uterus)
IT Uterus, metabolism
(of estrogens, model for)
IT Molecular structure-biological activity relationships
(uterus-binding, of estrogens)
IT 72-33-3 1035-77-4 **4954-12-5** 4954-14-7 7548-45-0
21507-16-4 21507-17-5 33526-45-3 33526-46-4 33526-47-5
33526-48-6 33713-12-1
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus)
IT 50-28-2, biological studies 57-63-6 21507-14-2 25918-89-2
RL: BIOL (Biological study)
(uterus binding of, estrogens effect on)
IT **4954-12-5**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

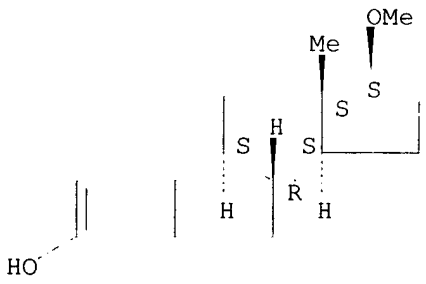
Absolute stereochemistry.



L65 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1970:432065 HCAPLUS

DN 73:32065
TI Action of natural, synthetic, and semisynthetic estrogens on deciduoma formation in rat uterus
AU Yoshino, Akio
CS Sch. Med., Jikei Univ., Tokyo, Japan
SO Tokyo Joshi Ika Daigaku Zasshi (1969), 84(5), 562-70
CODEN: TJIZAF
DT Journal
LA Japanese
CC 4 (Hormones and Related Substances)
AB Estrogens (I) priming action was examd. with natural synthetic and semisynthetic I on deciduoma formation in rat uterus and metabolism of phospholipid, cholesterol, and nucleic acid in decidual tissue. Female rats, weighing about 160 g, were used at 3 weeks after ovariectomy. Estrone, estradiol, estriol, estrone sulfate, estrone Me ether, estradiol Me ether, estrone benzoate, estradiol benzoate, ethynyl-estradiol, diethylstilbestrol, and hexestrol were used. The natural I were effective primers for the deciduoma formation in rat uterus; synthetic I did not have this action. Natural I had more effect on phospholipid and cholesterol metabolism in rat uterus than synthetic I. Natural and synthetic I showed effects on nucleic acid metabolism.
ST estrogens deciduoma uterus; deciduoma uterus estrogens; uterus deciduoma estrogens
IT Nucleic acids
Phospholipids
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus, estrogens effect on)
IT Uterus, metabolism
(of lipids and nucleic acids, estrogens effect on)
IT 50-27-1 50-28-2, biological studies 50-50-0 53-16-7, biological studies 56-53-1 57-63-6 481-97-0 1035-77-4 1624-62-0 2393-53-5 **4954-12-5** 5635-50-7
RL: BIOL (Biological study)
(lipid and nucleic acid metabolism by uterus in response to)
IT 57-88-5, biological studies
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus, estrogens effect on)
IT **4954-12-5**
RL: BIOL (Biological study)
(lipid and nucleic acid metabolism by uterus in response to)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

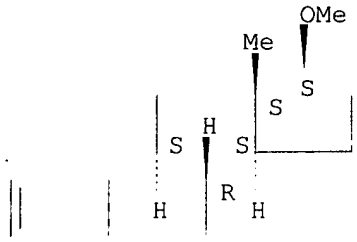
Absolute stereochemistry.



L65 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2002 ACS
AN 1969:477753 HCAPLUS
DN 71:77753
TI Mechanism of estrogen action in relation to carcinogenesis

AU Jensen, Elwood V.
CS Univ. of Chicago, Chicago, Ill., USA
SO Proc. Can. Cancer Res. Conf. (1966), Volume Date 1964, 6, 143-65
CODEN: PCCRA4
DT Journal
LA English
CC 4 (Hormones)
AB cf. CA 57:6523d. When 3H-labeled estradiol (I) or 17.alpha.-methylestradiol (II) was given s.c. in saline to Sprague-Dawley rats, absorption was rapid and the level of radioactivity in the blood and nonresponsive tissues reached a max. in 15 min., then fell rapidly, while the uterus and vagina continued to incorporate and retain radioactivity. When I or II was given s.c. in sesame oil, the levels in liver and nonresponsive tissues paralleled that in the blood, but in the uterus, vagina, anterior pituitary, and 7,12-dimethylbenz(a)anthracene - induced mammary tumors, there was a progressive uptake and retention. With hexestrol (III), retention in the vagina and uterus was more prolonged. The affinity of the uterus for estriol (IV) was not as striking as for I, but there was some retention in the growth-responsive tissues. The uterus and vagina showed no special affinity for estrone (V). Most of the uterine radioactivity after I administration was in the myometrium. The highest concn. of radioactivity was in the lamina propria with the radioactivity decreasing from the inner to outer myometrium. I was not readily taken up and retained by epithelial cells. After the administration of 0.1 .mu.g. I, II, or IV, all the radioactivity in the uterus and vagina was in the free steroid fraction after 15 min., 2 hrs., or 6 hrs., resp.; the same was observed in the 2 hr. uteri of III-treated animals. With V, free steroid predominated in the uterus, with some water-sol. radioactivity, but the liver and blood contained radioactivity bound to the alc.-insol. fraction and in the water-sol. form. After administration of I, II, or III, only I, II, or III appeared in the uterus and vagina, while injected IV appeared in the uterus as IV with small amts. of other polar steroids. After V administration, V was present in the uterus after 15 min. but after 2 hrs. V was gone and I was present. Metabolic transformation of I, II, and III occurred in the liver, but I, II, and III evidently stimulate growth in the rat uterus without undergoing metabolic transformation. An early if not initial step in the physiol. action of estrogenic hormones is an assocn. with receptor sites present in the uterus, vagina, and anterior pituitary. Interaction does not involve covalent bonds but is strong enough in vivo to permit the uptake and retention of steroid against a concn. gradient. The initial assocn. of estrogen with receptor sites was inhibited by estrogen antagonists like U-11100 and MER-25 but not actinomycin D or puromycin.
ST estrogens mechanism; mechanism estrogens; metab estrogens
IT Estrogenic hormones
RL: BIOL (Biological study)
(carcinogenesis in relation to)
IT Neoplasms, metabolism
(of estrogens in induced mammary)
IT 50-27-1 50-28-2, biological studies **4954-12-5** 5635-50-7
RL: BIOL (Biological study)
(in reproductive tract of female after administration)
IT **4954-12-5**
RL: BIOL (Biological study)
(in reproductive tract of female after administration)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

=> fil hcaold
FILE 'HCAOLD' ENTERED AT 11:46:26 ON 29 MAY 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

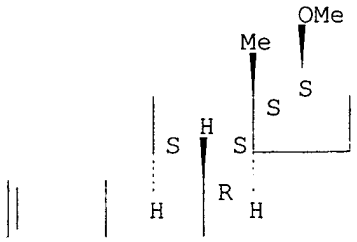
This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d all hitstr tot l64

L64 ANSWER 1 OF 3 HCAOLD COPYRIGHT 2002 ACS
AN CA64:8257g CAOLD
TI 17.beta.-estradiol 17-methyl ether
AU Coombs, M. M.; Roderick, H. R.
TI orientation of the fragmentation in mass spectrometry by the introduction of functional groups - (VII) ethylene ketals of 2-oxosteroids
AU Audier, Henri; Fetizon, M.; Gramain, J. C.
IT 700-77-6 1743-60-8 4832-17-1 4953-96-2 **4954-12-5**
4954-13-6 4954-14-7 4954-16-9 4954-17-0 4967-93-5 4967-94-6
4967-96-8 4967-97-9 4968-11-0 4999-72-8 5380-79-0 5506-56-9
6857-86-9
IT **4954-12-5**
RN 4954-12-5 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

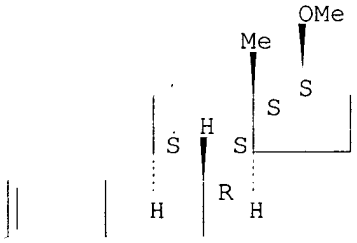
Absolute stereochemistry.



HO

L64 ANSWER 2 OF 3 HCAOLD COPYRIGHT 2002 ACS
AN CA61:16379g CAOLD
TI fractionation of estrogen methyl esters with Al2O3 column chromatography-estn. of of 16-epiestriol in pregnancy urine
AU Shida, Keizo; Kimura, N.; Kambegawa, A.
IT 1474-53-9 3434-79-5 **4954-12-5**
IT **4954-12-5**
RN 4954-12-5 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

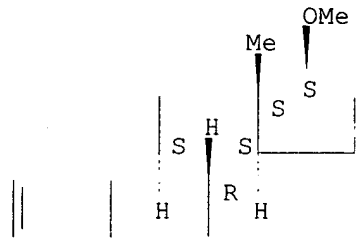
Absolute stereochemistry.



HO

L64 ANSWER 3 OF 3 HCAOLD COPYRIGHT 2002 ACS
AN CA56:7630a CAOLD
TI steroid derivs. - (XII) chromatography of neutral steroids on a thin Al2O3 layer
AU Hermanek, Stanislav; Schwarz, V.; Cekan, Z.
IT 113-38-2 604-32-0 633-34-1 809-51-8 1061-54-7 1169-49-9
1175-12-8 1182-65-6 1235-98-9 1255-57-8 1259-22-9 1639-43-6
1639-44-7 1807-15-4 2080-86-6 2088-71-3 2099-26-5 3604-60-2
4139-90-6 4651-48-3 4860-15-5 **4954-12-5** 6252-45-5
14072-39-0 14546-23-7 19637-35-5 20272-84-8 20867-15-6 23838-12-2
29163-23-3 29789-88-6 31823-53-7 33854-98-7 34209-81-9 41329-03-7
50303-03-2 71205-59-9 82979-88-2 95557-72-5 95908-73-9 96273-79-9
96275-23-9 96345-96-9 96391-62-7 96553-92-3 96772-72-4 107158-49-6
IT **4954-12-5**
RN 4954-12-5 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO

=> d all tot

L68 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS
AN 1966:44062 HCAPLUS
DN 64:44062
OREF 64:**8257f-g**
TI 17.beta.-Estradiol 17-methyl ether
AU Coombs, M. M.; Roderick, H. R.
CS Imp. Cancer Res. Fund, Lincoln's Inn Fields, London
SO Steroids (1965), 6(6), 841-4
DT Journal
LA English
CC 42 (Steroids)
AB Exptl. results and characterization of various products of 17.beta.-estradiol 17-Me ether are presented.

L68 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS
AN 1964:493831 HCAPLUS
DN 61:93831
OREF 61:**16379g-h**
TI Fractionation of estrogen methyl esters and alumina column chromatography (estimation of 16-epiestriol in pregnancy urine)
AU Shida, K.; Kimura, M.; Kanbegawa, A.
CS Med. and Dental Univ. School Med., Tokyo
SO Nippon Naibumpi Gakkai Zasshi (1961), 37(1), 5-9
DT Journal
LA Unavailable
CC 58 (Hormones)
AB After boiling for 15 min. with 15% concd. HCl, late pregnancy urine was extd. twice with ether, washed with 5% NaHCO3 and water, dried with anhyd. Na2SO4, and concd, to about 10 ml. in a water bath. The estrogens were extd. with benzene-petr. ether and reextd. with 1.6% NaOH. H3BO3 and dimethyl sulfate were added followed by stirring for 30 min. Following the addn. of 30% H2O2 the methylated estrogens were chromatographed on an alumina column 0.5 .times. 20 cm. prepd. by partial filling with petr. ether and the addn. of 2.0 g. of Brockmann alumina at 18.degree. under 10-12 mm. Hg. The Me esters of estrone, estradiol, 16-epiestriol, and estriol were eluted with 40% petr. ether in benzene, 1.0% MeOH in benzene, and 3.0% MeOH in benzene, resp. The content of 16-epiestriol reached 11.5% in late pregnancy urine. From Abstr. Japan. Med. 1(15), Abstr. No. 6640(1961).

L68 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
AN 1962:40001 HCAPLUS
DN 56:40001
OREF 56:**7630a-d**
TI Steroid derivatives. XII. Chromatography of neutral steroids on a thin aluminum oxide layer

AU Hermanek, S.; Schwarz, V.; Cekan, Z.
CS Research Inst. Nat. Drugs, Prague
SO Collection Czechoslov. Chem. Communs. (1961), 26, 1669-79
DT Journal
LA German
CC 55 (Biochemical Methods)
AB cf. CA 55, 27411c; 56, No. 5.-The use of Al2O3 without binder has the advantage of simplicity in prepg. a thin layer for chromatography. Alk. Al2O3 was used with ligroin (b. 30-50.degree.), benzene, ligroinbenzene, and benzene-EtOH mixts. in various proportions. .DELTA.4-3-Ketones were detected by lightly spraying with SbCl3 in CHCl3, other .DELTA.4-substances with SbCl3 in CHCl3 with 10% SOCl2. Alky. of Al2O3 was without influence on Rf values and, except for formates, trichloroacetates, and trifluoroacetates, did not degrade the substances during the 10-20 min. of development. Benzene was used as the first solvent for unknown mixts. Rf values in several solvents are tabulated for some 90 steroids belonging to 3-substituted cholest-5-enes, 17-substituted 3.beta.-acetoxyandrost-5-enes, 3.beta.substituted androst-5-en-17-ones, 3.beta.-substituted methyl-7keto-eti-5-enates, 3.beta.-substituted cholest-5-en-7-ones, 17.beta.substituted androst-4-en-3-ones, and miscellaneous classes. Chromatographic control of prepn. and purity of a substance is exemplified by the sepn. of pregn-4-ene-17.alpha.,21-diol-3,20-dione, its diacetates, 17.alpha.,21-diacetoxypregn-5-en3.beta.-ol-20-one, and 17.alpha.,21-diacetoxy-3.beta.-formyloxypregn-5en-20-one and accompanying impurities. Adsorptivity of 17.beta.-substituents increased in the following order: COOCH3, OBz, CN-COCH3, OAc, O, OH; for 3.beta.-substituents of cholest-5-ene the order was: H, Cl, OCH3, OAc, OH, and NMe2; similarly, cyclohexylamine moved more slowly than cyclohexanol while aniline was much faster than PhOH.

=> d his

(FILE 'REGISTRY' ENTERED AT 11:09:26 ON 29 MAY 2002)
DEL HIS

FILE 'HCAPLUS' ENTERED AT 11:09:34 ON 29 MAY 2002
E PROKAI L/AU
L1 89 S E3,E4
L2 1 S E7
E SIMPKINS J/AU
L3 227 S E3,E5,E7-E9
L4 22 S L1-L3 AND STERO?/SC,SX,CW
L5 123 S L1-L3 AND (?ESTROGEN? OR ?ESTRADIOL? OR ?STEROID?)
L6 126 S L4,L5
L7 8 S L1,L2 AND L3
L8 3 S L7 AND L4-L6
L9 0 S L6 AND ALKYLETHER
L10 2 S L6 AND ALKYL(L)ETHER
L11 2 S L10 AND L1-L10
SEL RN

FILE 'REGISTRY' ENTERED AT 11:12:06 ON 29 MAY 2002
L12 18 S E1-E18
L13 16 S L12 AND NR>=4
L14 5 S L13 AND (C22H32O2 OR C24H36O2 OR C26H40O2)
L15 3 S L14 NOT 3()(BUTOXY OR OCTYLOXY)
L16 777 S (C22H32O2 OR C24H36O2 OR C26H40O2)/MF AND C5-C6-C6-C6/ES
L17 110 S L16 AND 4432.3.65/RID AND 4/NR
L18 104 S L17 NOT 3 OL
L19 6 S L17 NOT L18
L20 5 S L19 NOT 13C#
L21 5 S L15,L20

```
                SEL RN
L22           0 S E19-E23/CRN

     FILE 'HCAOLD' ENTERED AT 11:20:06 ON 29 MAY 2002
L23           0 S L21

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:20:07 ON 29 MAY 2002
L24           1 S L21

     FILE 'HCAPLUS' ENTERED AT 11:20:18 ON 29 MAY 2002
L25           8 S L21
L26           3 S L1-L3 AND L25
L27           8 S L25,L26

     FILE 'REGISTRY' ENTERED AT 11:20:53 ON 29 MAY 2002

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:21:06 ON 29 MAY 2002

     FILE 'HCAPLUS' ENTERED AT 11:21:16 ON 29 MAY 2002

     FILE 'REGISTRY' ENTERED AT 11:21:39 ON 29 MAY 2002
L28             STR
L29           0 S L28 SAM
L30             STR L28
L31          21 S L30 SAM
L32        4506 S L30 FUL
                SAV TEMP L32 QAZI893324/A
L33        3917 S L32 AND 4432.3.65/RID
L34         589 S L32 NOT L33
L35             STR L28
L36           5 S L35 CSS SAM SUB=L32
L37         642 S L32 NOT ESTRA?
L38         314 S L37 NOT ?PREGN?/CNS
L39          86 S L38 NOT GONA?
L40          48 S L39 NOT CHOL?
L41        3864 S L32 NOT L37-L40
L42           3 S L32 NOT CN/FA
L43           5 S L35 CSS SAM SUB=L41
L44         100 S L35 CSS FUL SUB=L41
                SAV TEMP L44 QAZI893324A/A
L45          95 S L44 NOT L21
L46          93 S L45 NOT (ION OR LABELED OR (D OR T)/ELS OR 11C# OR 13C# OR 14
L47          22 S L46 AND 4/NR
L48           3 S L47 AND (C21H28O2 OR C21H26O2 OR C21H30O2)
L49             STR L35
L50           0 S L49 CSS SAM SUB=L32
L51          15 S L49 CSS FUL SUB=L32
                SAV L51 TEMP QAZI893324B/A
L52          13 S L51 NOT (13C# OR T/ELS)
L53           8 S L48,L52 NOT L21

     FILE 'HCAOLD' ENTERED AT 11:38:33 ON 29 MAY 2002
L54           0 S L53

     FILE 'HCAPLUS' ENTERED AT 11:38:36 ON 29 MAY 2002
L55          10 S L53

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:38:41 ON 29 MAY 2002
L56           1 S L53

     FILE 'REGISTRY' ENTERED AT 11:38:55 ON 29 MAY 2002

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:39:21 ON 29 MAY 2002
```

```
     FILE 'HCAPLUS' ENTERED AT 11:39:34 ON 29 MAY 2002
L57            25 S L32 AND L1-L3
                  SEL HIT RN

     FILE 'REGISTRY' ENTERED AT 11:40:22 ON 29 MAY 2002
L58            41 S E24-E64
L59            37 S L58 NOT L21,L53
L60            23 S L59 NOT (ESTER OR OATE)
L61            18 S L60 NOT CARBOXYLATE
L62            14 S L61 NOT ?OATE?/CNS
L63            11 S L62 NOT (ACETATE OR 17 17 DIMETHOXY)

     FILE 'HCAOLD' ENTERED AT 11:45:14 ON 29 MAY 2002
L64             3 S L63

     FILE 'HCAPLUS' ENTERED AT 11:45:28 ON 29 MAY 2002
L65            17 S L63

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:45:34 ON 29 MAY 2002
L66             4 S L63

     FILE 'REGISTRY' ENTERED AT 11:45:42 ON 29 MAY 2002

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:45:59 ON 29 MAY 2002

     FILE 'HCAPLUS' ENTERED AT 11:46:09 ON 29 MAY 2002

     FILE 'HCAOLD' ENTERED AT 11:46:26 ON 29 MAY 2002
                  SEL AN L64
                  EDIT /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 11:47:03 ON 29 MAY 2002
L67             6 S E65-E67
L68             3 S L67 NOT (AUDIER H? OR FUTTERWEIT W? OR SANNO Y?)/AU
```